

## WEST Search History

DATE: Wednesday, June 21, 2006

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		<i>DB=PGPB; PLUR=YES; OP=ADJ</i>	
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END OF SEARCH HISTORY

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 \*\*\*\*\* STN Columbus \*\*\*\*\*

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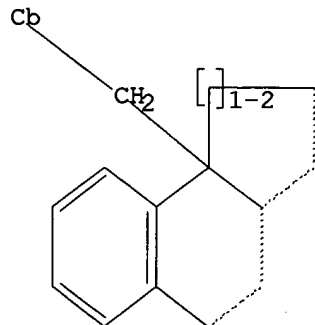
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L1 STRUCTURE UPLOADED

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L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 sam

L2 8 SEA SSS SAM L1

=> s l1 full

L3 901 SEA SSS FUL L1

=> file caplus

=> s l3

L4 89 L3

=> s l4 and pd< april 1999

19824199 PD< APRIL 1999

(PD<19990400)

L5 40 L4 AND PD< APRIL 1999

=> dis l5 1-40 bib abs hitstr

L5 ANSWER 1 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1999:812631 CAPLUS

DN 132:165996

TI Mechanochemical arylation and alkylation of fullerene C60 under the solvent-free conditions

AU Tanaka, Toru; Komatsu, Koichi

CS Institute for Chemical Research, Kyoto University, Kyoto, 611-0011, Japan

SO Synthetic Communications (1999), 29(24), 4397-4402

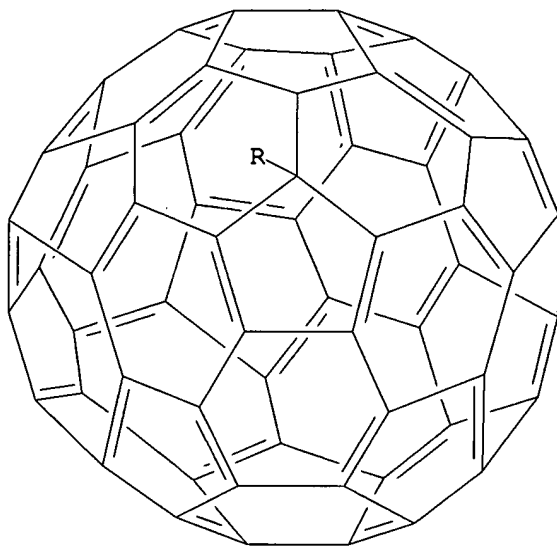
CODEN: SYNCAV; ISSN: 0039-7911

PB Marcel Dekker, Inc.

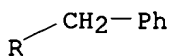
DT Journal

LA English  
 OS CASREACT 132:165996  
 AB The mechanochem. reaction of fullerene C60 with organic bromides and alkali metals gave the corresponding aryl or alkyl C60 derivs. under the solvent-free conditions.  
 IT **170646-75-0P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (mechanochem. arylation and alkylation of fullerene C60 under solvent-free conditions)  
 RN 170646-75-0 CAPLUS  
 CN [5,6]Fullerene-C60-1h, 1,9-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1999:735295 CAPLUS  
 DN 132:137266  
 TI Tandem nucleophilic addition/Diels - Alder reaction of N-butadienyl N,O-Ketene silyl acetals with C60: stereoselective formation of bicyclic octahydroquinolino-1,2,3,4-tetrahydrobuckminsterfullerenes and combined NMR spectroscopic and computational evaluation of the functionalization reactions  
 AU Rubin, Yves; Ganapathi, Padma S.; Franz, Andreas; An, Yi-Zhong; Qian, Wenyuan; Neier, Reinhard  
 CS Department of Chemistry and Biochemistry, University of California. Los Angeles, Los Angeles, CA, 90095-1569, USA

SO Chemistry--A European Journal (1999), 5(11), 3162-3184  
 CODEN: CEUJED; ISSN: 0947-6539

PB Wiley-VCH Verlag GmbH

DT Journal

LA English

OS CASREACT 132:137266

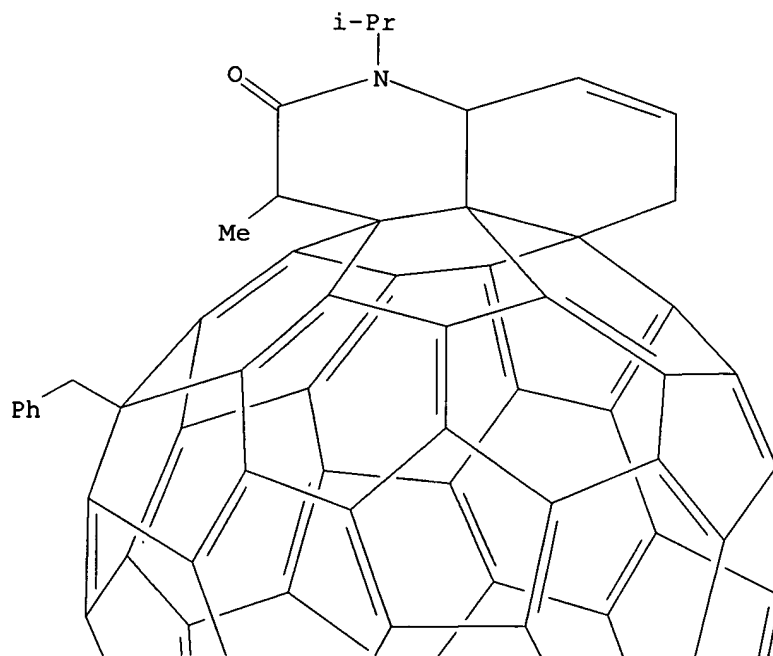
AB We have studied the reactivity of N,O-ketene N-1,3-butadienyl-N-alkyl-O-silyl acetals (Z)-RCH:CH(OSiMe<sub>2</sub>CMe<sub>3</sub>)N(R<sub>1</sub>)CH:CHCH:CH<sub>2</sub> (R = Me<sub>2</sub>CH, PhCH<sub>2</sub>, 9-anthracenylmethyl, 4-MeOC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>; R<sub>1</sub> = Me, 4-MeOC<sub>6</sub>H<sub>4</sub>, H<sub>2</sub>C:CH) (I) with C<sub>60</sub> proceeding through a tandem process to give tricyclic octahydroquinolinyl fullerene adducts. Deprotonation of the tricyclic octahydroquinolinyl fullerene adducts with sodium hydride and addition of alkylating agents such as Me iodide, allyl bromide, or benzyl bromide yield adducts alkylated on the fullerene. The addition order of these tandem reactions has been evaluated. The initial nucleophilic Michael-like addition of I proceeds unusually fast at 25°C, followed by an intramolecularly accelerated Diels - Alder step that is highly diastereoselective. The structures of the tricyclic octahydroquinolinyl fullerene adducts were determined from the <sup>1</sup>H and <sup>13</sup>C NMR shifts and from H - H coupling patterns, while their stereochem. was deduced from 2D T-ROESY NMR expts. The proposed mechanism for the nucleophilic addition involves single electron transfer followed by radical anion - radical cation recombination. Computational investigations of the reaction pathways, transition states, and conformational energies have been carried out to corroborate the exptl. data.

IT **256652-27-4P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of fullerene derivs. by deprotonation of octahydroquinolinyl fullerenes and addition of electrophiles)

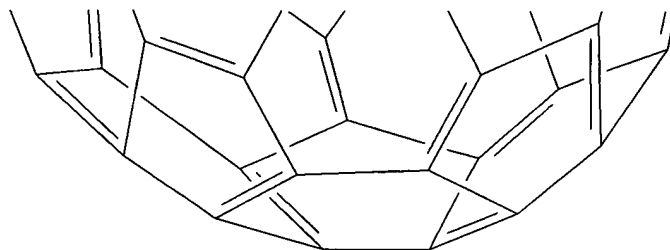
RN 256652-27-4 CAPLUS

CN 1'H,14H-[5,6]Fullereno-C<sub>60</sub>-1h-[2,1,9-de]quinolin-2'(3'H)-one,  
 6',8'a-dihydro-3'-methyl-1'-(1-methylethyl)-14-(phenylmethyl)-,  
 stereoisomer (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



RE.CNT 157 THERE ARE 157 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1999:654258 CAPLUS  
DN 131:315178  
TI Electrosynthesis and characterization of (C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>4</sub>C<sub>60</sub> isomers  
AU Kadish, Karl M.; Gao, Xiang; Van Caemelbecke, Eric; Suenobu, Tomoyoshi;  
Fukuzumi, Shunichi  
CS Department of Chemistry, University of Houston, Houston, TX, 77204-5641,  
USA  
SO Proceedings - Electrochemical Society (1999), 99-12 (Recent  
Advances in the Chemistry and Physics of Fullerenes and Related  
Materials), 92-114  
CODEN: PESODO; ISSN: 0161-6374  
PB Electrochemical Society

DT Journal

LA English

AB The structural, spectral, and electrochem. properties of 2 (C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>4</sub>C<sub>60</sub> isomers are reported. One is designated as the 1,4,1,4-(C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>4</sub>C<sub>60</sub> isomer and the other as the 1,4,1,2-isomer of (C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>4</sub>C<sub>60</sub>. The 1,4,1,2-isomer is the first example of an organofullerene possessing both 1,4- and 1,2-addition patterns. The 2 isomers were isolated by HPLC from the products produced in a reaction between the dianion of (C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>2</sub>C<sub>60</sub> and C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>Br. X-ray data show that the 2 organofullerenes differ from one another by the position of only 1 benzyl group with the 4 benzyl substituents being in close proximity to each other in each compound. Both (C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>4</sub>C<sub>60</sub> isomers undergo 3 one-electron redns. in PhCN containing 0.1 M tetra-n-butylammonium perchlorate (TBAP) and have E<sub>1/2</sub> values which are more neg. than those of either C<sub>60</sub> or 1,4-(C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>2</sub>C<sub>60</sub>. The monoanions of 1,4,1,4- and 1,4,1,2-(C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>4</sub>C<sub>60</sub> were electrogenerated by bulk controlled-potential electrolysis in PhCN containing 0.2 M TBAP and characterized as to their spectral properties in both the visible and near IR regions.

IT **207684-63-7**

RL: RCT (Reactant); RACT (Reactant or reagent)  
(in electrosynthesis of (C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>4</sub>C<sub>60</sub> isomers)

RN 207684-63-7 CAPLUS

CN [5,6]Fullerene-C<sub>60</sub>-Ih, 1,2,3,13-tetrahydro-3,13-bis(phenylmethyl)-, ion(2-) (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

IT **247185-05-3 247185-06-4**

RL: PRP (Properties)  
(spectral data of monoanions of (C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>4</sub>C<sub>60</sub> isomers prepared by electrosynthesis)

RN 247185-05-3 CAPLUS

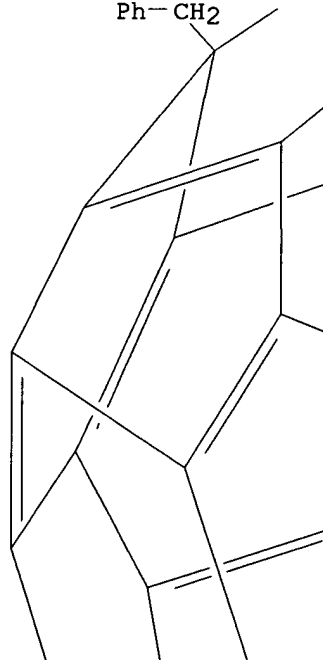
CN [5,6]Fullerene-C<sub>60</sub>-Ih, 1,6,11,18-tetrahydro-1,6,11,18-tetrakis(phenylmethyl)-, radical ion(1-) (9CI) (CA INDEX NAME)

PAGE 1-A

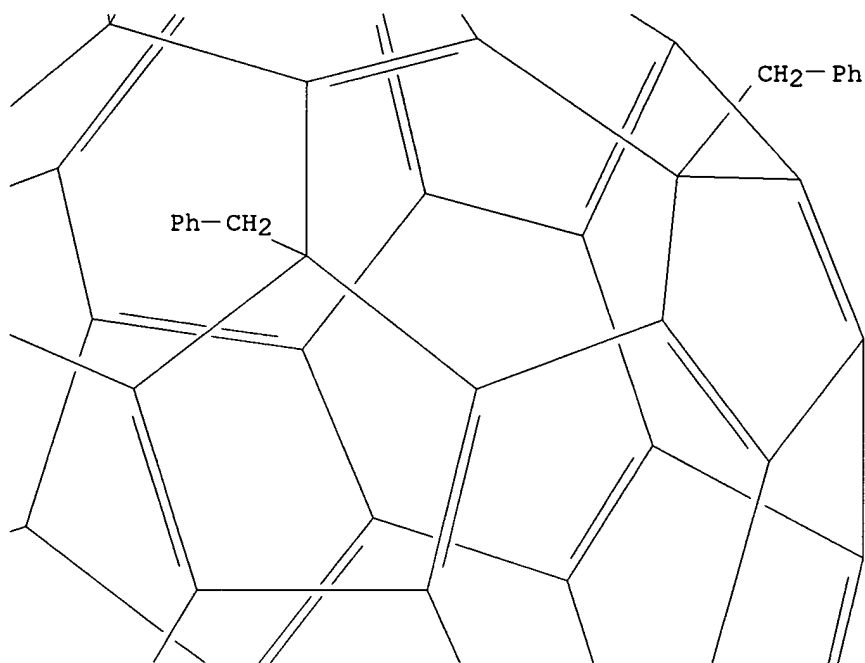
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PAGE 2-A  
Ph-CH<sub>2</sub>

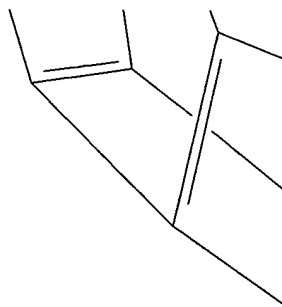


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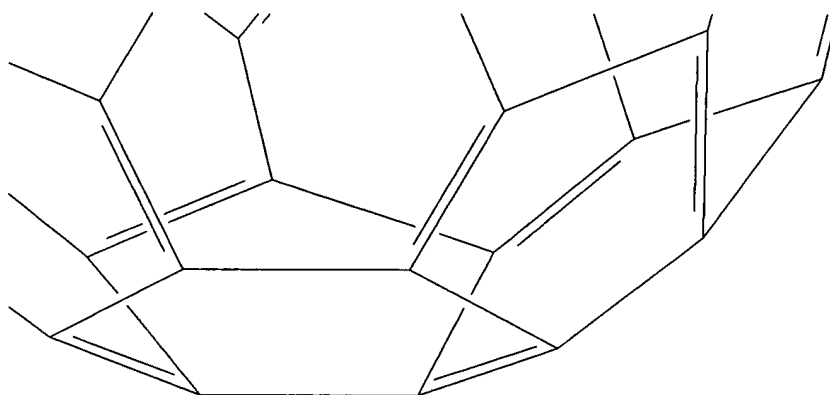




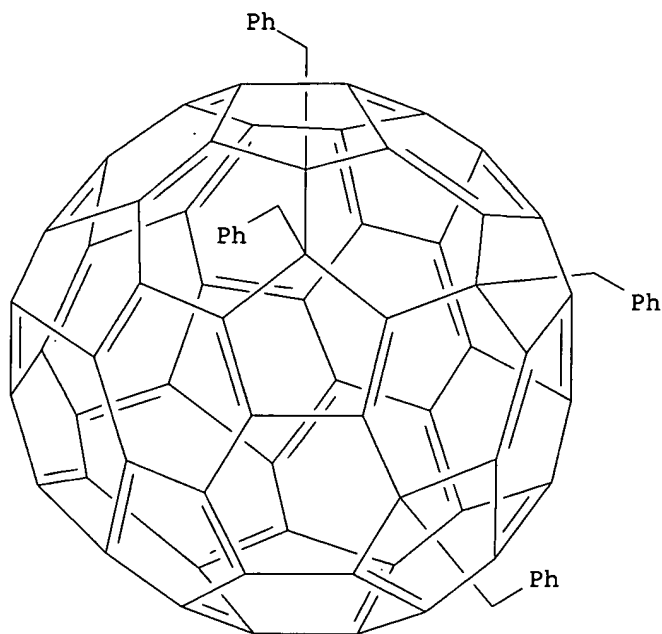
PAGE 3-A



PAGE 3-B



RN 247185-06-4 CAPLUS  
CN [5,6]Fullerene-C60-Ih, 1,6,9,18-tetrahydro-1,6,9,18-tetrakis(phenylmethyl)-  
, radical ion(1-) (9CI) (CA INDEX NAME)



IT **207684-64-8P 247185-87-1P**

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)  
(structural, spectral, and electrochem. properties of (C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>4</sub>C<sub>60</sub> isomers)

RN 207684-64-8 CAPLUS

CN [5,6]Fullerene-C<sub>60</sub>-I<sub>h</sub>, 1,6,11,18-tetrahydro-1,6,11,18-tetrakis(phenylmethyl)- (9CI) (CA INDEX NAME)

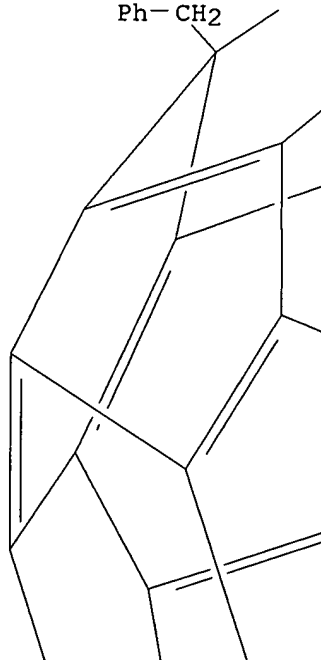
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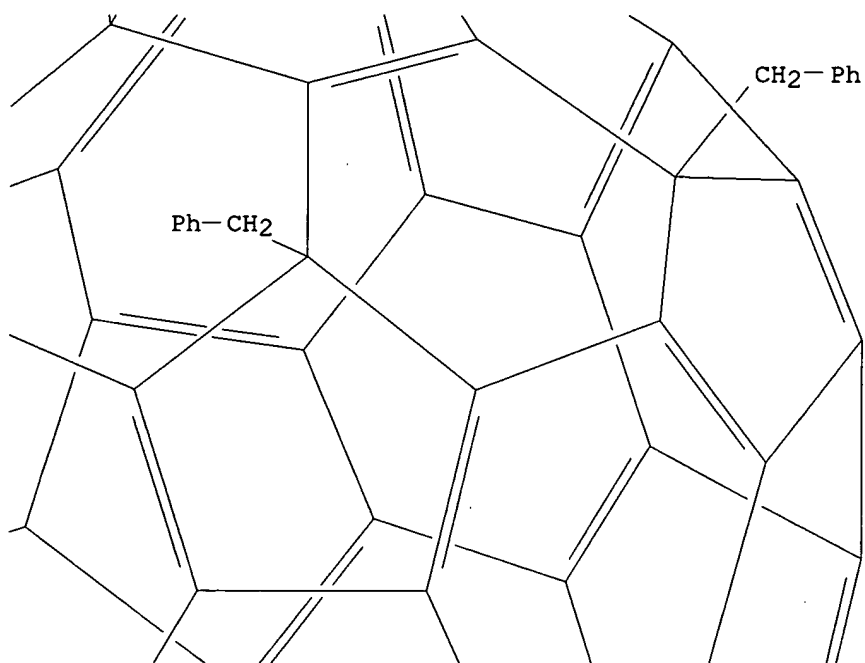
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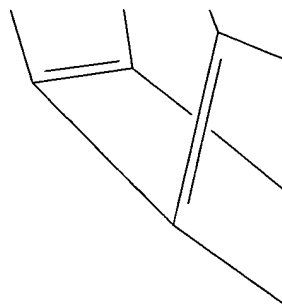
PAGE 2-A  
Ph-CH<sub>2</sub>



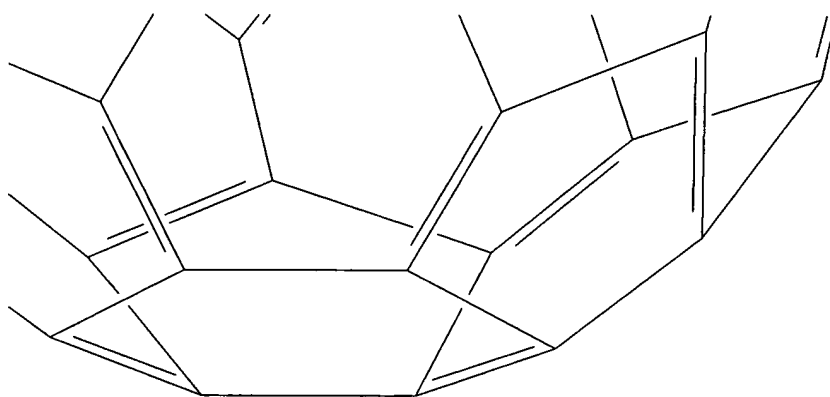
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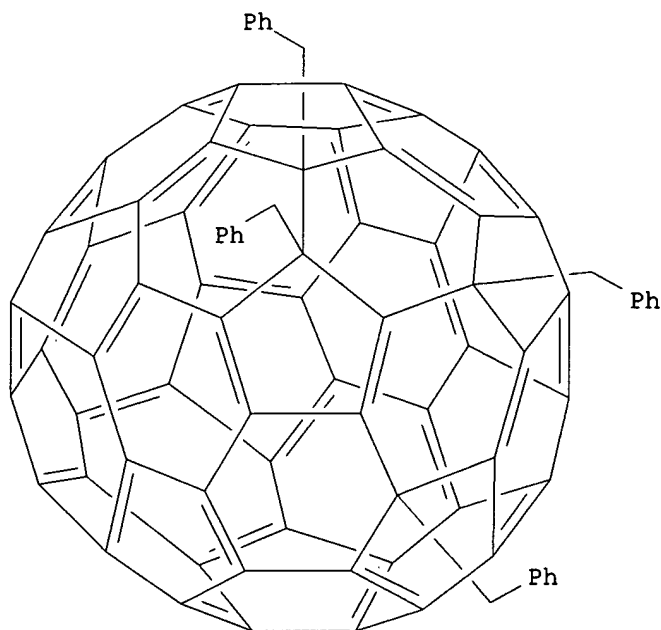
PAGE 3-A



PAGE 3-B



RN 247185-87-1 CAPLUS  
CN [5,6]Fullerene-C60-Ih, 1,6,9,18-tetrahydro-1,6,9,18-tetrakis(phenylmethyl)-  
(9CI) (CA INDEX NAME)



RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1999:560721 CAPLUS

DN 131:350971

TI Radical functionalization of [60]fullerene and its derivatives initiated by the  $C(CF_3)_2C_6H_4F$  radical

AU Tumanskii, B. L.; Kalina, O. G.; Bashilov, V. V.; Usatov, A. V.; Shilova, E. A.; Lyakhovetskii, Yu. I.; Solodovnikov, S. P.; Bubnov, N. N.; Novikov, Yu. N.; Lobach, A. S.; Sokolov, V. I.

CS A. N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Moscow, 117813, Russia

SO Russian Chemical Bulletin (Translation of Izvestiya Akademii Nauk, Seriya Khimicheskaya) (1999), 48(6), 1108-1112  
CODEN: RCBUEY; ISSN: 1066-5285

PB Consultants Bureau

DT Journal

LA English

AB It was found that the 2-(p-fluorophenyl)hexafluoroisopropyl radical produced by thermal dissociation of the Polishchuk dimer  $[C(CF_3)_2C_6H_4F]_2$  can withdraw, under mild conditions, the H atom from the Me group of toluene and mesitylene to form the corresponding radicals, whose addition to [60]fullerene occurs more selectively than in the case of photochem. production of these radicals. Dynamics of the step-by-step multiaddn. of the radicals to  $C_{60}$  was studied by ESR. It was found that the addition of benzyl radicals affords adducts containing from 3 to 5 benzyl groups, whereas no spin-adducts with five addends were observed for more bulky 3,5-dimethylphenylmethyl radicals. The interaction of 3,5-dimethylphenylmethyl radicals with the metal complexes  $(\eta^2-C_{60})[IrH(CO)(PPh_3)_2]$  and  $(\eta^2-C_{60})[Pd(PPh_3)_2]$  was studied for the first time. It was shown that the palladium derivative undergoes only demetalation. In the case of the Ir complex, up to 3 radicals add to the

fullerene ligand in the same hemisphere where the transition metal is coordinated. The reaction rates are .apprx.5 times lower than those for C60. The ability of 2-(p-fluorophenyl)hexafluoroisopropyl radicals to dehydrogenate C60H36 was found.

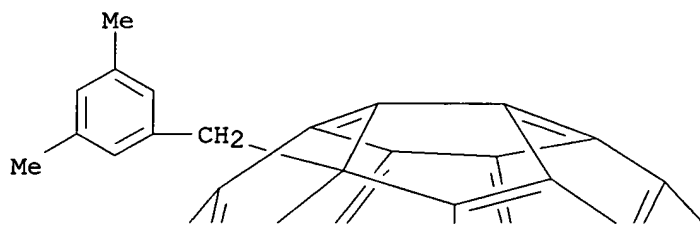
IT 245476-77-1

RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)  
(radical functionalization of [60]fullerene and its organometallic  
derivs. initiated by the C(CF3)2C6H4F-p radical)

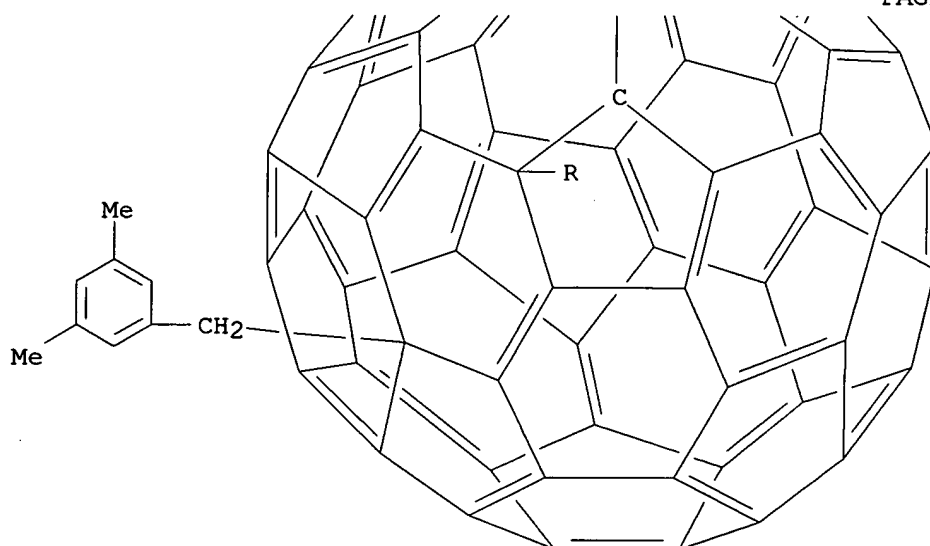
RN 245476-77-1 CAPLUS

CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 2,10,14-tris[(3,5-dimethylphenyl)methyl]-  
10,14-dihydro- (9CI) (CA INDEX NAME)

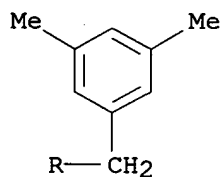
PAGE 1-A



PAGE 2-A

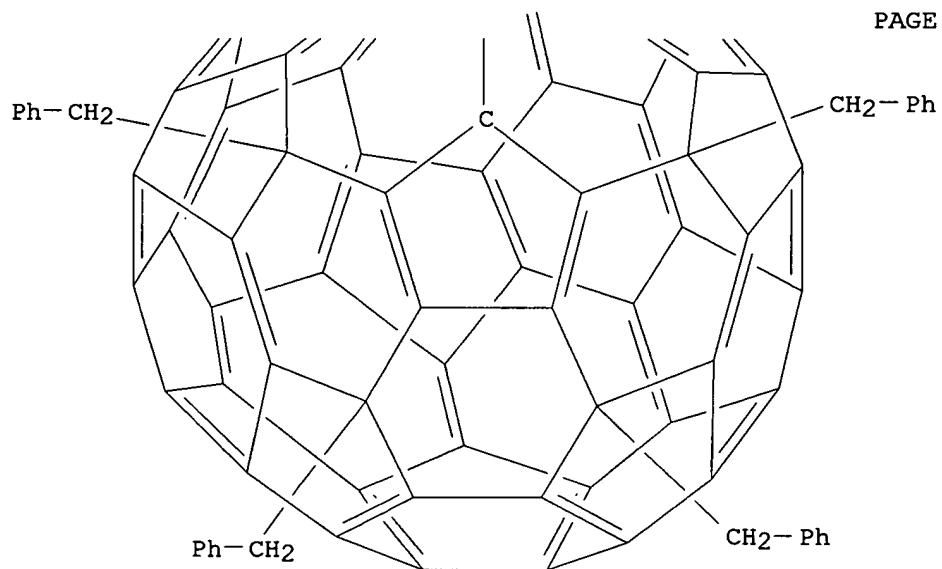
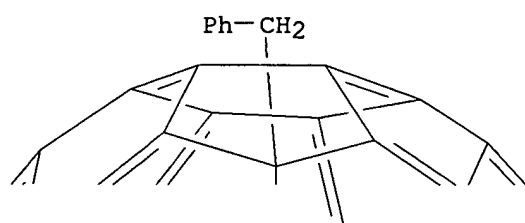


PAGE 3-A



IT **139141-78-9 140700-29-4 250671-55-7**  
 RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM  
 (Formation, nonpreparative); RACT (Reactant or reagent)  
 (radical functionalization of [60]fullerene and its organometallic  
 derivs. initiated by the C(CF<sub>3</sub>)<sub>2</sub>C<sub>6</sub>H<sub>4</sub>F-p radical)  
 RN 139141-78-9 CAPLUS  
 CN [5,6]Fulleren-C<sub>60</sub>-1h-1(9H)-yl, 6,12,15,18-tetrahydro-6,9,12,15,18-  
 pentakis(phenylmethyl)- (9CI) (CA INDEX NAME)





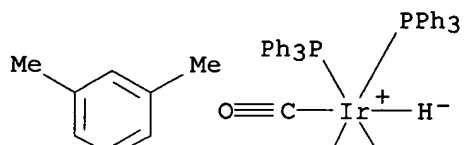
RN 140700-29-4 CAPLUS  
CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 10,14-dihydro-2,10,14-tris(phenylmethyl)-  
(9CI) (CA INDEX NAME)

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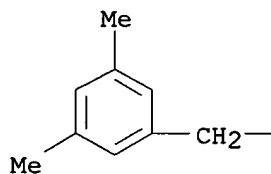
RN 250671-55-7 CAPLUS

CN Iridium, carbonyl[(3,15-η)-10,14-dihydro-2,10,14-tris[(3,5-dimethylphenyl)methyl][5,6]fulleren-C60-Ih-1(2H)-yl]hydrobis(triphenylphosphine)-, stereoisomer (9CI) (CA INDEX NAME)

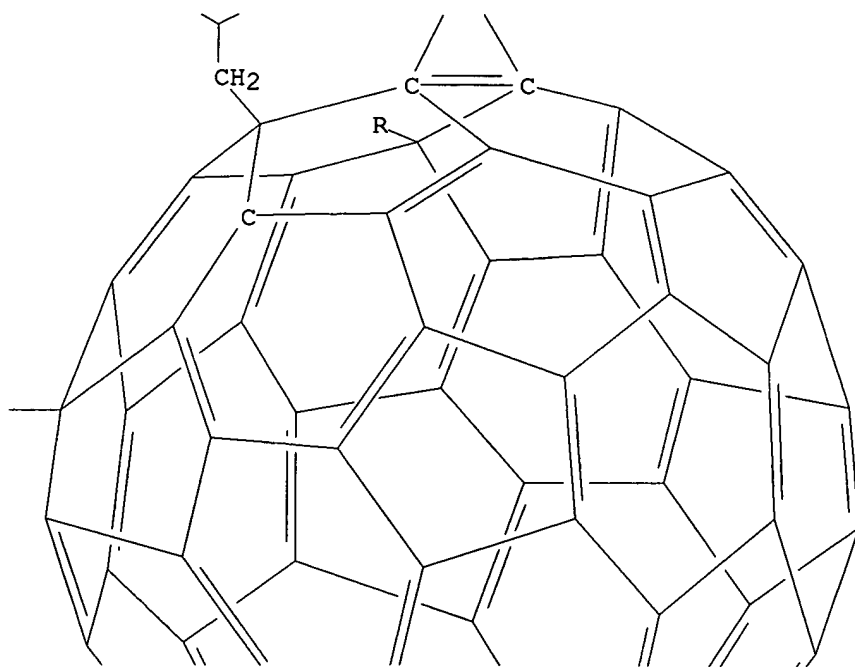
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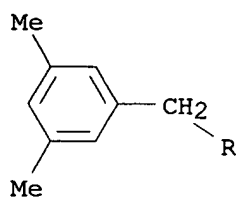
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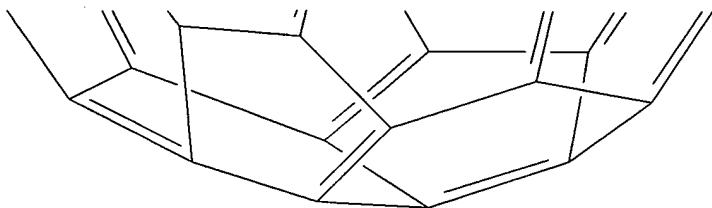


PAGE 2-B



PAGE 3-A

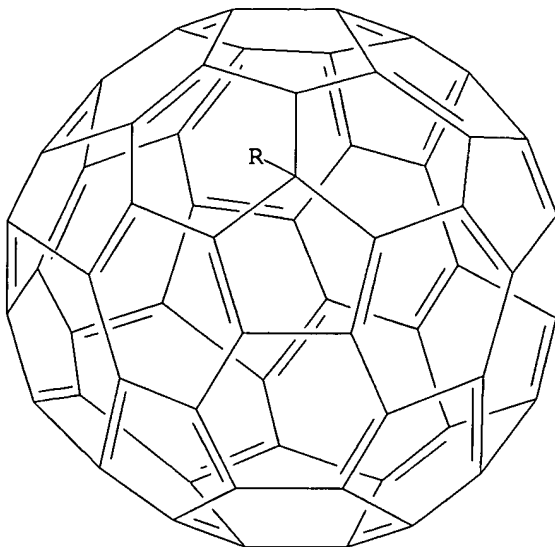




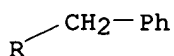
RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1999:392433 CAPLUS  
DN 131:129618  
TI [60]Fullerene radical cation: reactions and mechanism  
AU Siedschlag, Christina; Luftmann, Heinrich; Wolff, Christian; Mattay,  
Jochen  
CS Institut Organische Chemie, Christian-Albrechts-Universitat Kiel, Kiel,  
D-24098, Germany  
SO Tetrahedron (1999), 55(25), 7805-7818  
CODEN: TETRAB; ISSN: 0040-4020  
PB Elsevier Science Ltd.  
DT Journal  
LA English  
AB C60 was irradiated in the presence of several electron transfer  
photosensitizers. Upon addition of H-donors such as N,N-dimethylformamide,  
1,3-dioxolane, phenylacetaldehyde, Me formate, tert-butanol, propionic  
acid, glycol and methoxyethanol, 1-substituted 1,2-dihydro[60]fullerenes  
and in one case a 1,2,3,4-tetrahydro[60]fullerene were formed. A  
mechanistic pathway involving C60+ is proposed.  
IT **170646-75-0P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(mechanism of photoinduced electron transfer mediated addition of hydrogen  
donors to C60 fullerene)  
RN 170646-75-0 CAPLUS  
CN [5,6]Fullerene-C60-1h, 1,9-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX  
NAME)

PAGE 1-A



PAGE 2-A

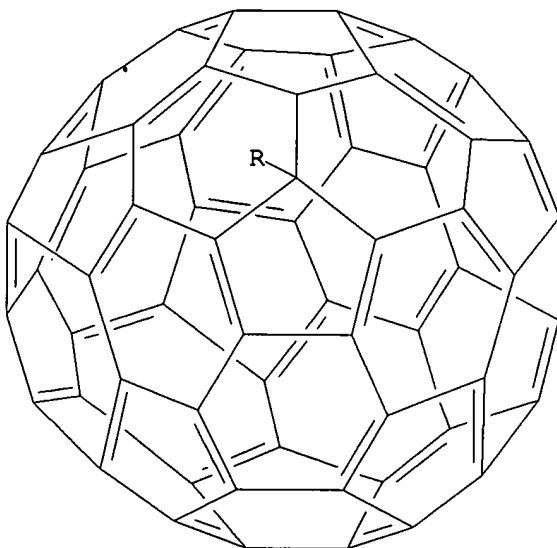


RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

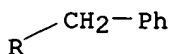
L5 ANSWER 6 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1999:251966 CAPLUS  
 DN 131:37660  
 TI Radical ions in fullerene chemistry  
 AU Siedschlag, Ch.; Torres-Garcia, G.; Wolff, Ch.; Mattay, J.; Fujitsuka, M.;  
 Watanabe, A.; Ito, O.; Dunsch, L.; Ziegs, F.; Luftmann, H.  
 CS Institut für Organische Chemie, Universität Kiel, Kiel, D-24098, Germany  
 SO Journal of Information Recording (1998), 24(3-4), 265-270  
 CODEN: JIREFL; ISSN: 1025-6008  
 PB Gordon & Breach Science Publishers  
 DT Journal  
 LA English  
 AB [60]Fullerene is irradiated in the presence of several electron transfer  
 photosensitizers. Upon addition of various H-donors 1-substituted  
 1,2-dihydro-[60]fullerenes are formed. Mechanistic studies using laser  
 flash photolysis as well as ESR spectroscopy reveal the formation of the  
 radical cation of [60]fullerene. In addition the [2 + 2]photoreactions of  
 4-methyl-1,2,4-triazoline-3,5-dione with [60]fullerene derivs. are  
 reported.  
 IT **170646-75-0P**  
 RL: PNU (Preparation, unclassified); PREP (Preparation)  
 (formation from fullerene by photolysis in presence of hydrogen donor  
 and electron transfer photosensitizer)  
 RN 170646-75-0 CAPLUS  
 CN [5,6]Fullerene-C60-Ih, 1,9-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX

NAME)

PAGE 1-A



PAGE 2-A



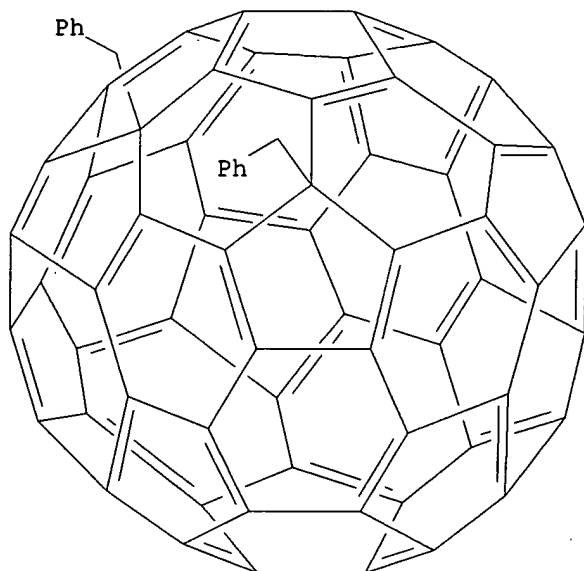
RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1998:638828 CAPLUS  
 DN 129:330532  
 TI Alkylation of C60<sup>2-</sup> generated from C60H<sub>2</sub>  
 AU Meier, Mark S.; Bergosh, Robert G.  
 CS Department of Chemistry, University of Kentucky, Lexington, KY,  
 40506-0055, USA  
 SO Proceedings - Electrochemical Society (1998), 98-8 (Recent  
 Advances in the Chemistry and Physics of Fullerenes and Related  
 Materials), 1103-1109  
 CODEN: PESODO; ISSN: 0161-6374  
 PB Electrochemical Society  
 DT Journal  
 LA English  
 AB The preparation of mono- and dialkylfullerenes from C60H<sub>2</sub> is reported.  
 Deprotonation of C60H<sub>2</sub> with tetrabutylammonium hydroxide in benzonitrile  
 generates C60<sup>2-</sup> dianion, which reacts rapidly with selected alkyl halides.  
 Alkylation is successful when the alkylating agent can generate relatively  
 stable radicals. Tosylates are unreactive in both the first and second  
 alkylation step. The monoalkylated fullerenes were obtained as  
 1,2-regioisomers, while dialkylfullerenes were obtained as 1,4  
 regioisomers.  
 IT 176106-61-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (selective mono- and dialkylation of C60<sup>2-</sup> generated from C60H<sub>2</sub>)

RN 176106-61-9 CAPLUS

CN [5,6]Fullerene-C60-1h, 1,7-dihydro-1,7-bis(phenylmethyl)- (9CI) (CA INDEX NAME)



RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 8 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1998:569500 CAPLUS

DN 129:244749

TI Formation of C60 Adducts with Two Different Alkyl Groups via Combination of Electron Transfer and SN<sub>2</sub> Reactions

AU Fukuzumi, Shunichi; Suenobu, Tomoyoshi; Hirasaka, Takeomi; Arakawa, Ryuichi; Kadish, Karl M.

CS Department of Material and Life Science Graduate School of Engineering, Osaka University, Suita Osaka, 565-0871, Japan

SO Journal of the American Chemical Society (1998), 120(36), 9220-9227

CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

LA English

OS CASREACT 129:244749

AB The formation of organofullerenes of the type R<sub>2</sub>C<sub>60</sub> and R(R')C<sub>60</sub> from C<sub>60</sub><sup>2-</sup> and alkyl halides (RX or R'X) in benzonitrile was mechanistically investigated for 15 different alkyl halides which vary in electrophilicity and electron acceptor ability. The first step in the reaction leads to RC<sub>60</sub><sup>-</sup> via an electron-transfer mechanism, followed by formation of R<sub>2</sub>C<sub>60</sub> or R(R')C<sub>60</sub> via an SN<sub>2</sub> mechanism. Evidence of the mechanism comes from comparison of rate consts. for the stepwise addition of two R groups to C<sub>60</sub><sup>2-</sup> with rate consts. for the genuine electron transfer and SN<sub>2</sub> reactions. The formation of t-BuC<sub>60</sub><sup>-</sup> and PhCH<sub>2</sub>C<sub>60</sub><sup>-</sup> after the first R group addition was confirmed by electrospray ionization mass spectroscopy. The t-BuC<sub>60</sub><sup>-</sup>

derivative will not react further with excess t-BuI, but this is not the case for the less sterically hindered PhCH<sub>2</sub>Br, which adds to t-BuC<sub>60</sub><sup>-</sup> in benzonitrile to give t-Bu(PhCH<sub>2</sub>)C<sub>60</sub>. A protonation of t-BuC<sub>60</sub><sup>-</sup> with trifluoroacetic acid can also occur to give 1,4-t-Bu(H)C<sub>60</sub>, which rearranges rapidly to yield 1,2-t-Bu(H)C<sub>60</sub>. Rate consts. for the second alkylation of t-BuC<sub>60</sub><sup>-</sup> with a variety of different alkyl halides are compared with values of genuine S<sub>N</sub>2 reactions and indicate that the second step in the fullerene alkylation reaction proceeds via an S<sub>N</sub>2 mechanism. The rate consts. of electron transfer from C<sub>60</sub><sup>2-</sup> to RX span a range of 10<sup>5</sup>, but are insensitive to the steric effect of the alkyl group, i.e., they depend only on the electron-acceptor ability of RX. In contrast, the S<sub>N</sub>2 rate consts. of t-BuC<sub>60</sub><sup>-</sup> with RX are highly susceptible to the steric effect of the alkyl group and no reaction at all takes place between t-BuC<sub>60</sub><sup>-</sup> and t-BuI. Thus, the first addition of one sterically hindered alkyl group to C<sub>60</sub><sup>2-</sup> occurs via electron transfer and cannot be followed by further addition of a second sterically hindered group (via an S<sub>N</sub>2 reaction). This is not the case for less sterically hindered alkyl groups such as benzyl bromide which can add via an S<sub>N</sub>2 reaction to yield C<sub>60</sub> adducts with two different alkyl groups.

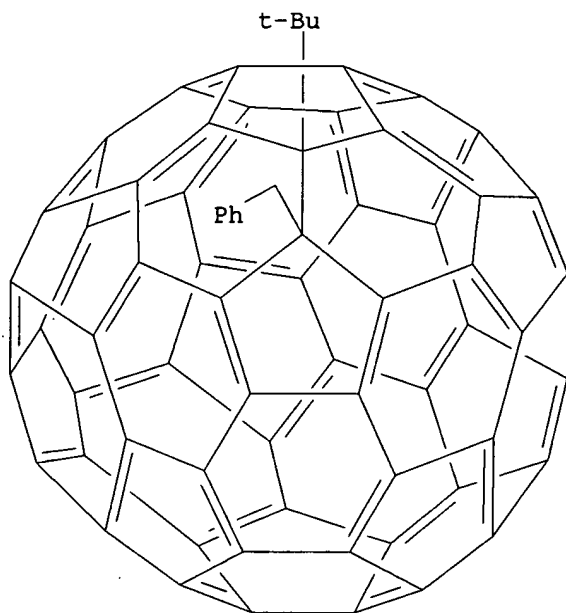
IT 195392-52-0

RL: PRP (Properties)

(calculated formation enthalpy; formation of C<sub>60</sub> adducts with two different alkyl groups via combination of electron transfer and S<sub>N</sub>2 reactions)

RN 195392-52-0 CAPLUS

CN [5,6]Fullerene-C<sub>60</sub>-1h, 1-(1,1-dimethylethyl)-1,9-dihydro-9-(phenylmethyl)-(9CI) (CA INDEX NAME)



IT 182070-59-3

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(formation of C<sub>60</sub> adducts with two different alkyl groups via combination of electron transfer and S<sub>N</sub>2 reactions)

RN 182070-59-3 CAPLUS

CN [5,6]Fullerene-C<sub>60</sub>-1h, 1,2-dihydro-1-(phenylmethyl)-, ion(1-) (9CI) (CA

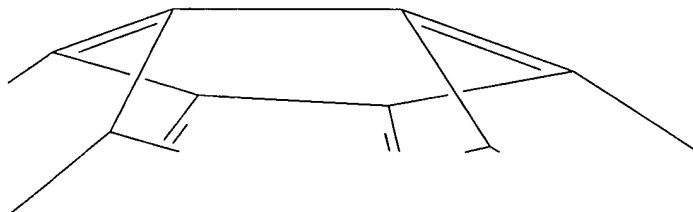


INDEX NAME)

PAGE 1-A



PAGE 1-B



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

IT **160482-48-4P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(formation of C60 adducts with two different alkyl groups via  
combination of electron transfer and SN2 reactions)

RN 160482-48-4 CAPLUS

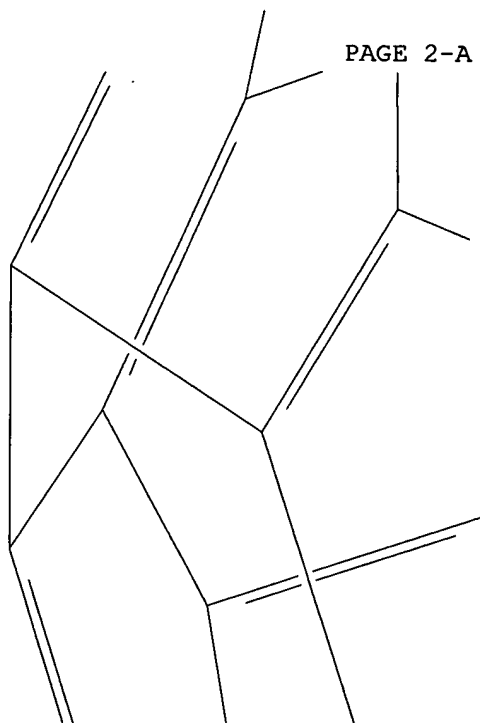
CN [5,6]Fullerene-C60-Ih, 1-(1,1-dimethylethyl)-1,7-dihydro-7-(phenylmethyl)-  
(9CI) (CA INDEX NAME)

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

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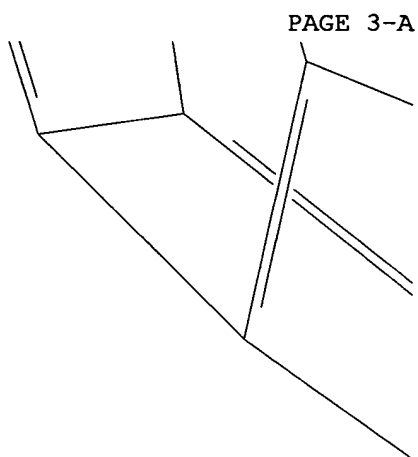
PAGE 1-C

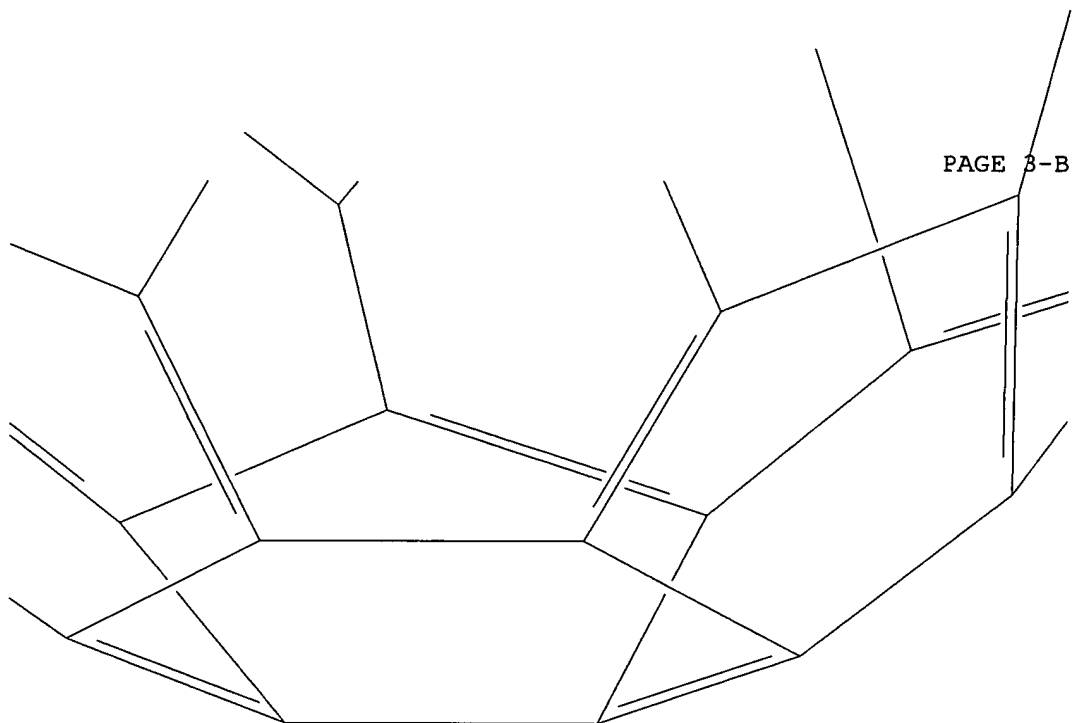




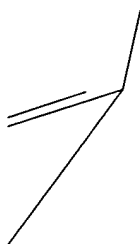
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*





PAGE 3-B



PAGE 3-C

RE.CNT 136 THERE ARE 136 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 9 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1998:499423 CAPLUS  
DN 129:195665  
TI Selective One-Electron and Two-Electron Reduction of C60 with NADH and NAD  
Dimer Analogs via Photoinduced Electron Transfer  
AU Fukuzumi, Shunichi; Suenobu, Tomoyoshi; Patz, Matthias; Hirasaka, Takeomi;  
Itoh, Shinobu; Fujitsuka, Mamoru; Ito, Osamu  
CS Department of Material and Life Science Graduate School of Engineering,  
Osaka University, Suita, Osaka, 565-0871, Japan  
SO Journal of the American Chemical Society (1998), 120(32),  
8060-8068  
CODEN: JACSAT; ISSN: 0002-7863  
PB American Chemical Society

DT Journal

LA English

AB The selective one-electron reduction of C60 to C60•- is attained through photoinduced electron transfer from an NADH analog, 1-benzyl-1,4-dihydronicotinamide (BNAH), and the dimer analog [(BNA)2] to the triplet excited state of C60. The limiting quantum yield for formation of C60•- in the case of (BNA)2 exceeds unity;  $\Phi_{\infty} = 1.3$ . In this case, the initial electron transfer from (BNA)2 to the triplet excited state (3C60\*) is followed by fast C-C bond cleavage in the resulting (BNA)2•+ to give BNA• and BNA+ and the second electron transfer from BNA• to C60 yields BNA+ and C60•-, when (BNA)2 acts as a two-electron donor to produce 2 equiv of C60•-. When BNAH is replaced by 4-tert-butylated BNAH (t-BuBNAH), the photochem. reaction with C60 yields not C60•- but instead the tert-butylated anion (t-BuC60-) selectively. In this case, the initial electron transfer from t-BuBNAH to 3C60\* is also followed by fast C-C bond cleavage in t-BuBNAH•+ to give t-Bu•, which is coupled with C60•- produced in the electron transfer to yield t-BuC60-. The selective two-electron reduction of C60 to 1,2-dihydro[60]fullerene (1,2-C60H2) is also attained with the use of another NADH analog, 10-methyl-9,10-dihydroacridine (AcrH2), under visible light irradiation in deaerated benzonitrile solution containing trifluoroacetic acid.

The studies on the quantum yields, the kinetic deuterium isotope effects, and the quenching of the triplet-triplet absorption of C60 by AcrH2 have revealed that the photochem. reduction proceeds via photoinduced electron transfer from 10-methyl-9,10-dihydroacridine to the triplet excited state of C60, which is followed by proton transfer from AcrH2•+ to C60•- and a second electron transfer from the deprotonated acridinyl radical (AcrH•) to C60H• in the presence of trifluoroacetic acid to yield the final products 10-methylacridinium ion (AcrH+) and 1,2-C60H2. The transient spectra of the radical ion pair formed in the photoinduced electron transfer have been detected successfully in laser flash photolysis of each NADH analog-C60 system. The mechanistic difference between the selective one- and two-electron redns. of C60 is discussed on the basis of the difference in the redox and acid-base properties of NADH and the dimer analogs.

IT 160482-48-4P

RL: PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

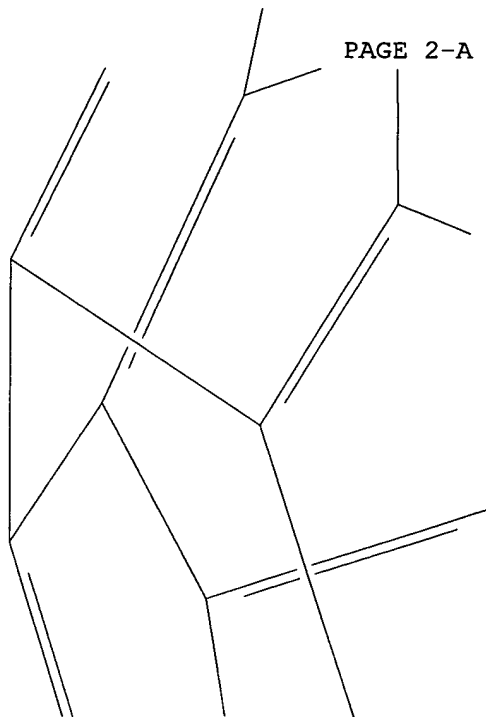
(selective one-electron and two-electron reduction of C60 with NADH and NAD dimer analogs via photoinduced electron transfer)

RN 160482-48-4 CAPLUS

CN [5,6]Fullerene-C60-1h, 1-(1,1-dimethylethyl)-1,7-dihydro-7-(phenylmethyl)-(9CI) (CA INDEX NAME)

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

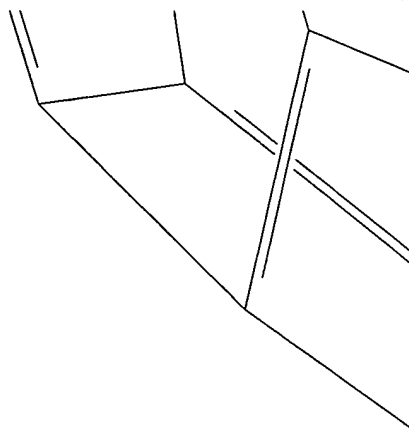
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*



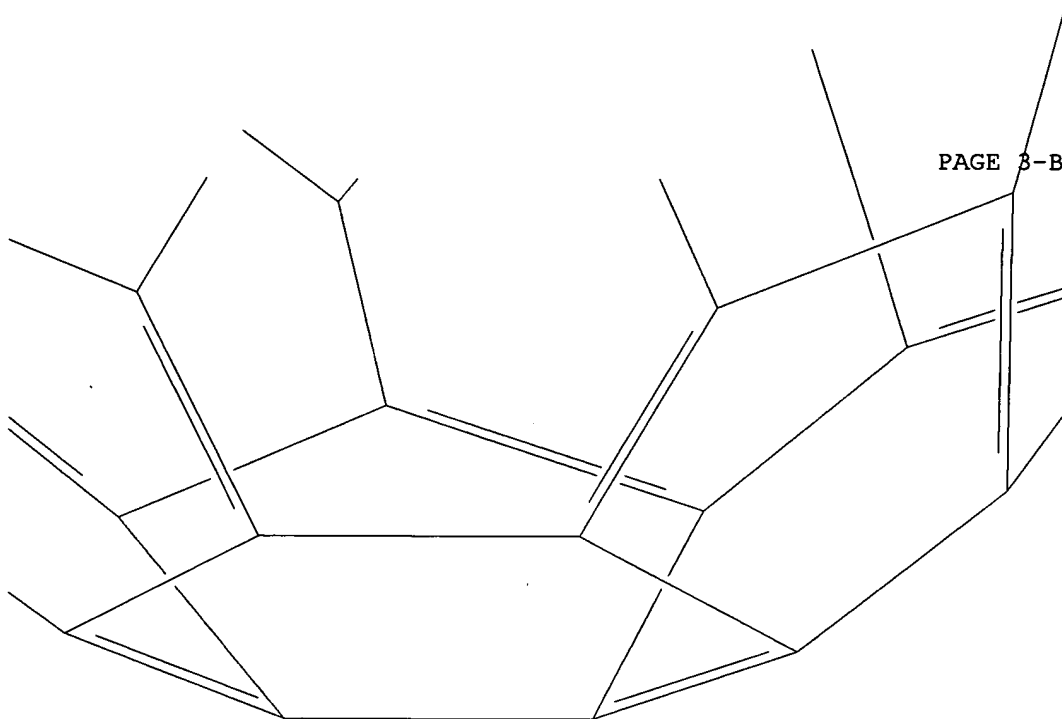
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

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PAGE 3-A



PAGE 3-B

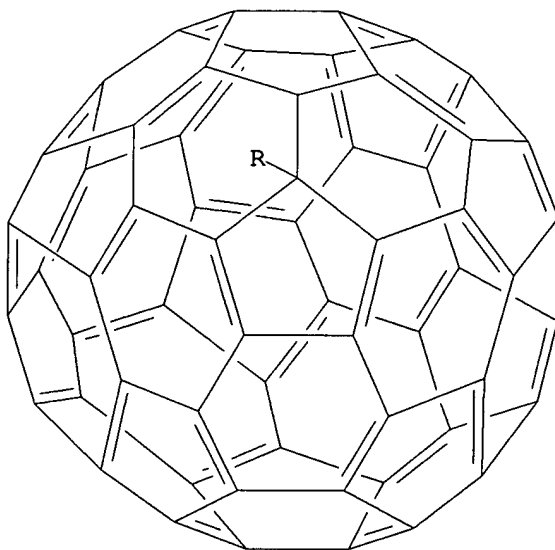


RE.CNT 77 THERE ARE 77 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

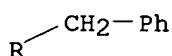
L5 ANSWER 10 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1998:439511 CAPLUS  
DN 129:208728  
TI Photoluminescence of fullerene [60] in ultrathin ordered multilayers: the dissociation of molecular aggregation  
AU Ma, Shihong; Lu, Xingze; Xu, Jianhua; Cai, Zhigang; Zhou, Jianying; Wang, Wencheng; Zhang, Zhiming  
CS State Key Joint Laboratory for Materials Modification by Laser, Ion and Electron Beams, Department of Physics, Fudan University, Shanghai, 200433, Peop. Rep. China  
SO Chinese Science Bulletin (1998), 43(12), 1004-1008  
CODEN: CSBUEF; ISSN: 1001-6538  
PB Science in China Press  
DT Journal  
LA English  
AB The aggregation behavior of a substituted fullerene compound, 1-benzyl-2-hydro[60]fullerene (C60-Be), in Z-type ultrathin ordered (e.g. LB) multilayers was studied by UV-visible absorption, steady state and time-resolved fluorescence spectroscopies. The LB multilayers of pure C60-Be showed J-aggregate formation, characterized by a large red shift of two absorption peaks ( $\Delta E$ .apprx.2,098 cm<sup>-1</sup> from 260→275 nm and  $\Delta E$ .apprx.1,076 cm<sup>-1</sup> from 328→340 nm, resp.). The main fluorescence emission bands were found at 710, 646, 603, 600 and 595 nm for pure C60-Be, mixed C60-Be (molar percentage 50%, 25% and 20%, resp.) multilayers and monomeric C60-Be, mixed C60-Be (molar percentage 50%, 25% and 20%, resp.) in LB films could be best-fitted by using a bi-exponential decay model.  
IT **170646-75-0**  
RL: OCU (Occurrence, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); OCCU (Occurrence); PROC (Process)  
(photoluminescence of fullerene [60] in ultrathin ordered multilayers and dissociation of mol. aggregation)  
RN 170646-75-0 CAPLUS  
CN [5,6]Fullerene-C60-Ih, 1,9-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX NAME)



PAGE 1-A



PAGE 2-A



RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 11 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1998:282928 CAPLUS  
DN 129:27672  
TI Synthesis and Spectroscopic and Electrochemical Characterization of Di- and Tetrasubstituted C60 Derivatives  
AU Kadish, Karl M.; Gao, Xiang; Van Caemelbecke, Eric; Hirasaka, Takeomi; Suenobu, Tomoyoshi; Fukuzumi, Shunichi  
CS Department of Chemistry, University of Houston, Houston, TX, 77204-5641, USA  
SO Journal of Physical Chemistry A (1998), 102(22), 3898-3906  
CODEN: JPCAFH; ISSN: 1089-5639  
PB American Chemical Society  
DT Journal  
LA English  
AB The synthesis and electrochem. and spectroscopic characterization of fullerene derivs. of the type R2C60 where R = C6H5CH2, 2-BrC6H4CH2, 3-BrC6H4CH2, or 4-BrC6H4CH2 and R4C60 where R = C6H5CH2 are reported. The first step in the synthesis involves an electron transfer between C602- and RBr, and a similar initial electron-transfer step occurs between [(C6H5CH2)2C60]2- and C6H5CH2Br during the synthesis of (C6H5CH2)4C60. On the basis of NMR and UV-visible data, the investigated R2C60 derivs. are identified as 1,4-adducts of C60, whereas the isolated isomer of (C6H5CH2)4C60 is characterized as possessing C1 symmetry with the four benzyl groups being close to each other. The electrochem. of each synthesized compound was determined in benzonitrile containing 0.1 M

tetra-n-butylammonium perchlorate and each mono- and dianion of R2C60 and R4C60 were characterized by near-IR spectroscopy. The near-IR spectra of each species show two major "marker bands" which can be considered to be diagnostic of the fullerene derivative oxidation state.

IT **207684-64-8**

RL: PRP (Properties)

(calculated LUMO structure; synthesis and spectroscopic and electrochem. characterization of di- and tetrabenzylated C60 derivs.)

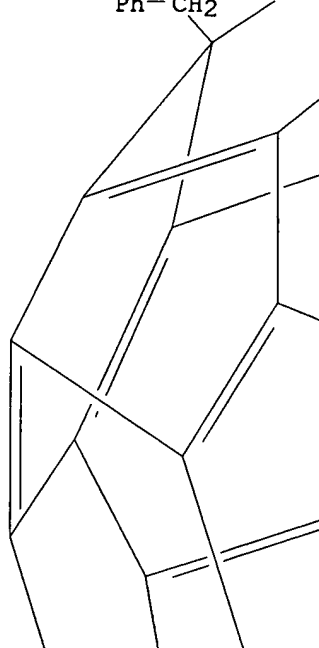
RN 207684-64-8 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,6,11,18-tetrahydro-1,6,11,18-tetrakis(phenylmethyl)- (9CI) (CA INDEX NAME)

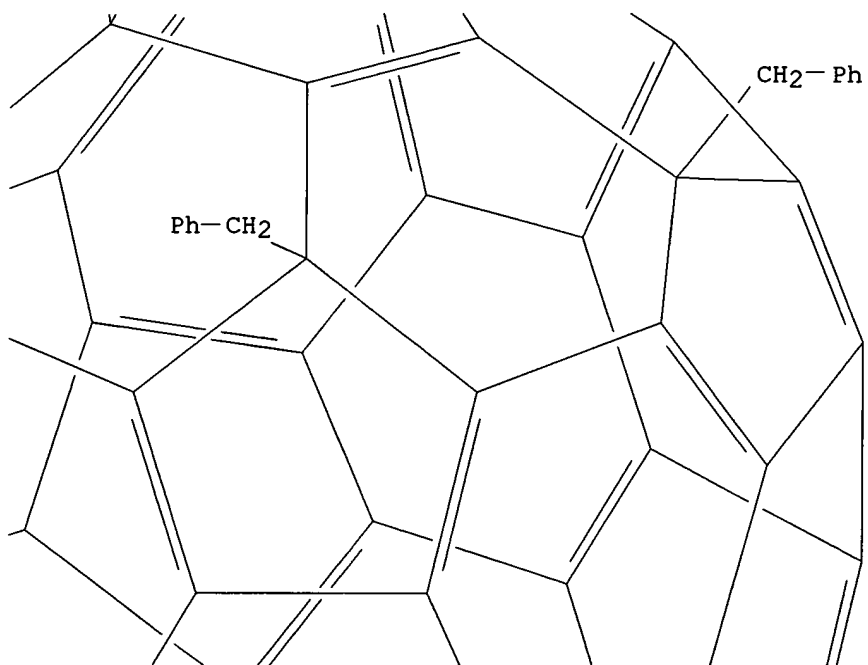
PAGE 1-A



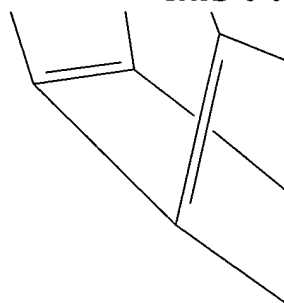
PAGE 2-A  
Ph-CH<sub>2</sub>

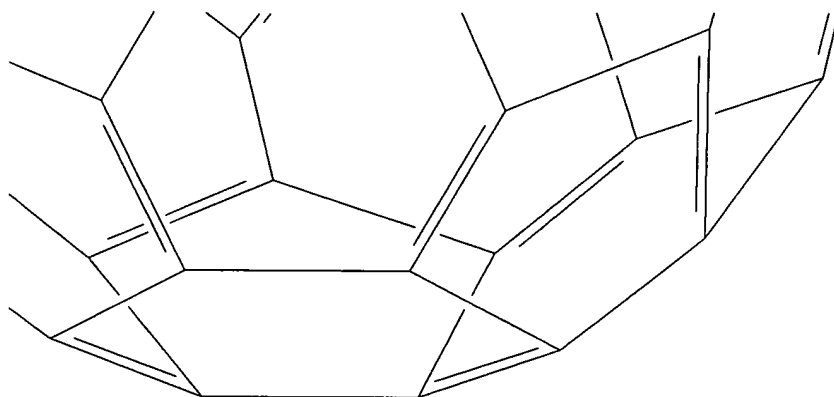


PAGE 2-B



PAGE 3-A





IT **207684-63-7**

RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)  
(synthesis and spectroscopic and electrochem. characterization of di- and tetrabenzylated C60 derivs.)

RN 207684-63-7 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,2,3,13-tetrahydro-3,13-bis(phenylmethyl)-, ion(2-) (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

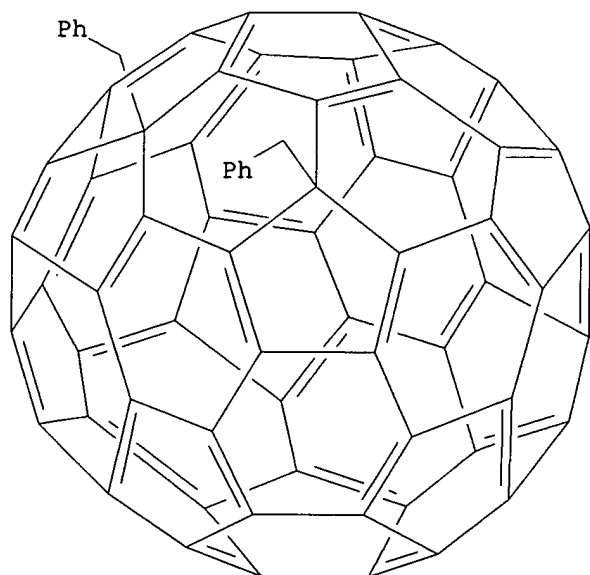
IT **182212-24-4 195625-44-6 195625-45-7  
195625-46-8 207684-65-9 207684-66-0  
207684-67-1**

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(synthesis and spectroscopic and electrochem. characterization of di- and tetrabenzylated C60 derivs.)

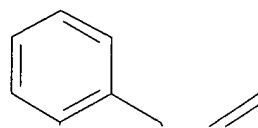
RN 182212-24-4 CAPLUS

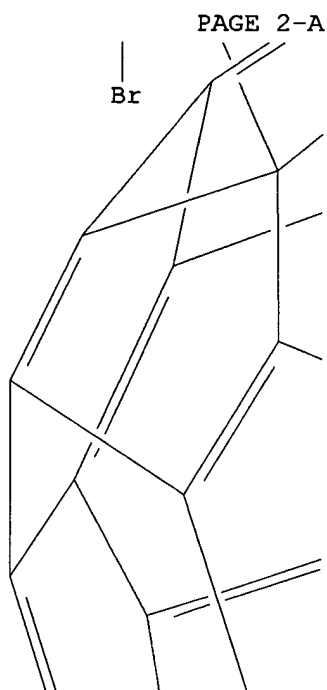
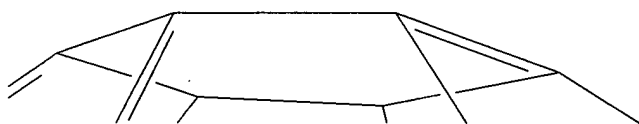
CN [5,6]Fullerene-C60-Ih, 1,7-dihydro-1,7-bis(phenylmethyl)-, radical ion(1-) (9CI) (CA INDEX NAME)



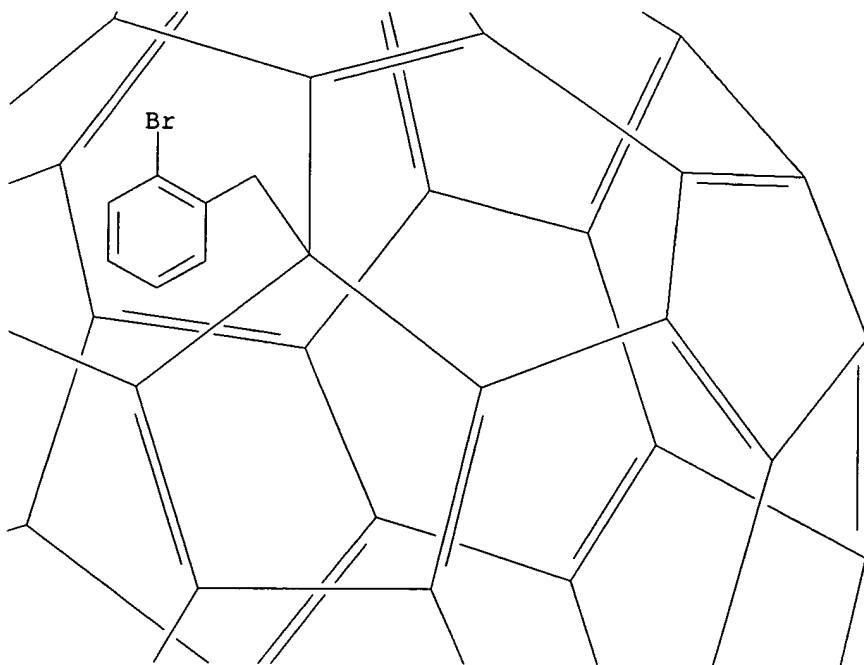
RN 195625-44-6 CAPLUS  
 CN [5,6]Fullerene-C60-1h, 1,7-bis[(2-bromophenyl)methyl]-1,7-dihydro-,  
 radical ion(1-) (9CI) (CA INDEX NAME)

PAGE 1-A

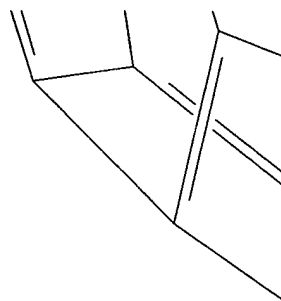




PAGE 2-B

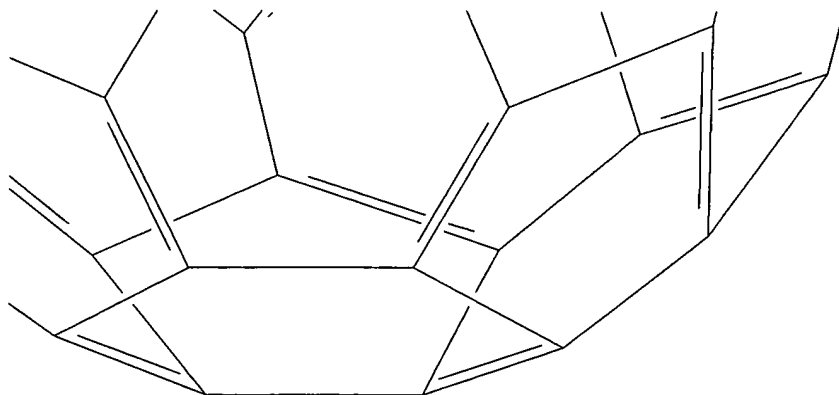


PAGE 3-A





PAGE 3-B



RN 195625-45-7 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-bis[(3-bromophenyl)methyl]-1,7-dihydro-,  
radical ion(1-) (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 195625-46-8 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-bis[(4-bromophenyl)methyl]-1,7-dihydro-,  
radical ion(1-) (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 207684-65-9 CAPLUS

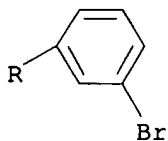
CN [5,6]Fullerene-C60-Ih, 3,13-bis[(2-bromophenyl)methyl]-1,2,3,13-tetrahydro-,  
ion(2-) (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

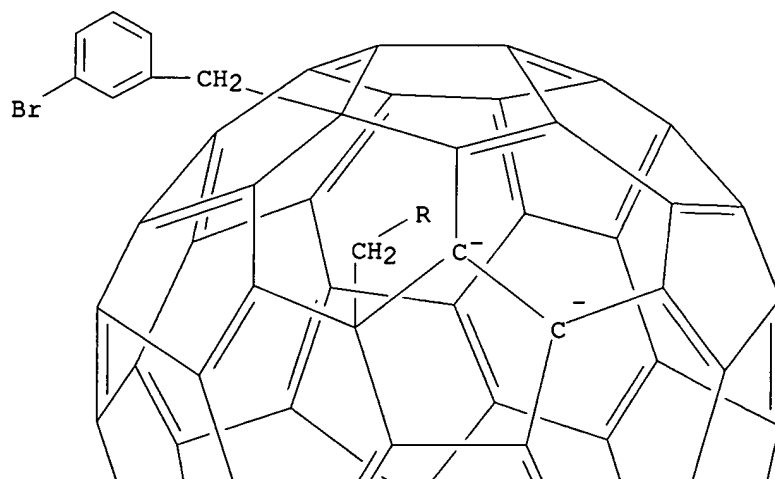
RN 207684-66-0 CAPLUS

CN [5,6]Fullerene-C60-Ih, 3,13-bis[(3-bromophenyl)methyl]-1,2,3,13-tetrahydro-,  
ion(2-) (9CI) (CA INDEX NAME)

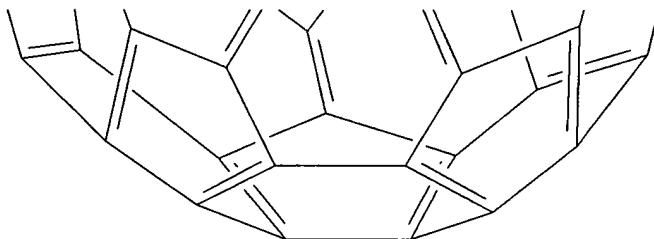
PAGE 1-A



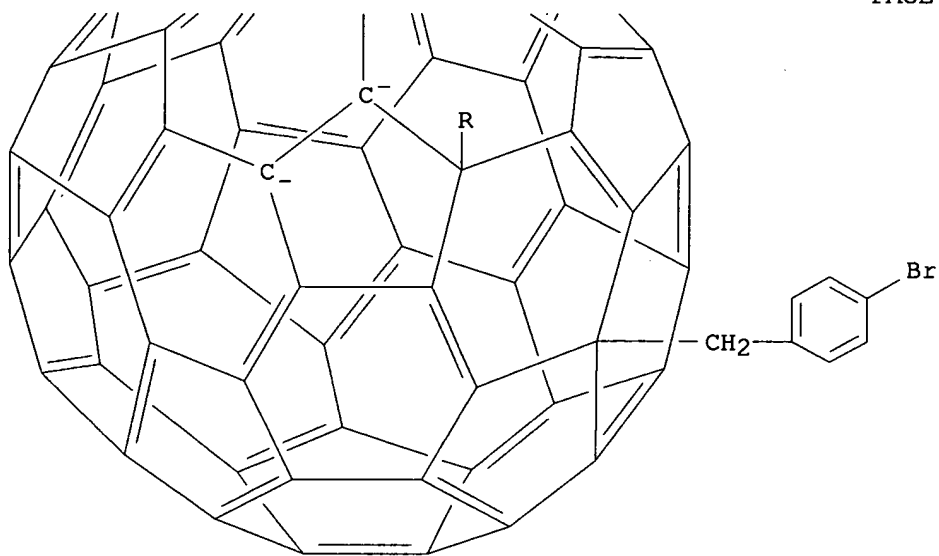
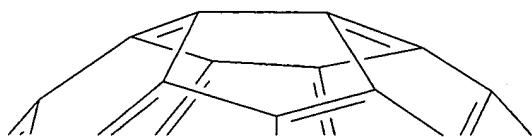
PAGE 2-A

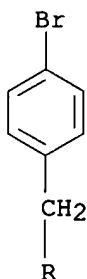


PAGE 3-A



RN 207684-67-1 CAPLUS  
 CN [5,6]Fullerene-C60-Ih, 3,13-bis[(4-bromophenyl)methyl]-1,2,3,13-tetrahydro-  
 , ion(2-) (9CI) (CA INDEX NAME)



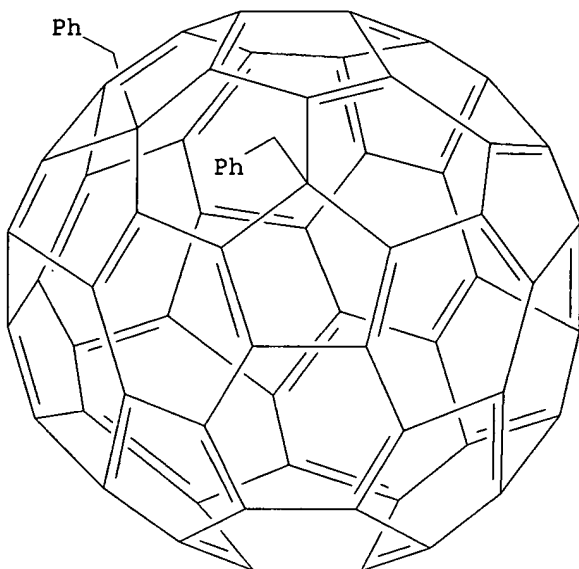


IT **176106-61-9P**

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)  
(synthesis and spectroscopic and electrochem. characterization of di- and tetrabenzylated C60 derivs.)

RN 176106-61-9 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-dihydro-1,7-bis(phenylmethyl)- (9CI) (CA INDEX NAME)



IT **195625-41-3P 195625-42-4P 195625-43-5P**

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(synthesis and spectroscopic and electrochem. characterization of di- and tetrabenzylated C60 derivs.)

RN 195625-41-3 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-bis[(2-bromophenyl)methyl]-1,7-dihydro- (9CI)  
(CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 195625-42-4 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-bis[(3-bromophenyl)methyl]-1,7-dihydro- (9CI)

(CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 195625-43-5 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-bis[(4-bromophenyl)methyl]-1,7-dihydro- (9CI)  
(CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RE.CNT 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 12 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1998:273225 CAPLUS

DN 129:40968

TI Synthesis and characterization of [(C6H5CH2)4C60]n- where n = 0, 1 or 2  
AU Gao, Xiang; Van Caemelbecke, Eric; Materazzi, Stefano; Kadish, Karl M.;  
Fukuzumi, Shunichi; Suenobu, Tomoyoshi; Hirasaka, TakeomiCS Department of Chemistry, University of Houston, Houston, TX, 77204-5641,  
USASO Proceedings - Electrochemical Society (1997), 97-42 (Recent  
Advances in the Chemistry and Physics of Fullerenes and Related Materials,  
Vol. 5), 99-116

CODEN: PESODO; ISSN: 0161-6374

PB Electrochemical Society

DT Journal

LA English

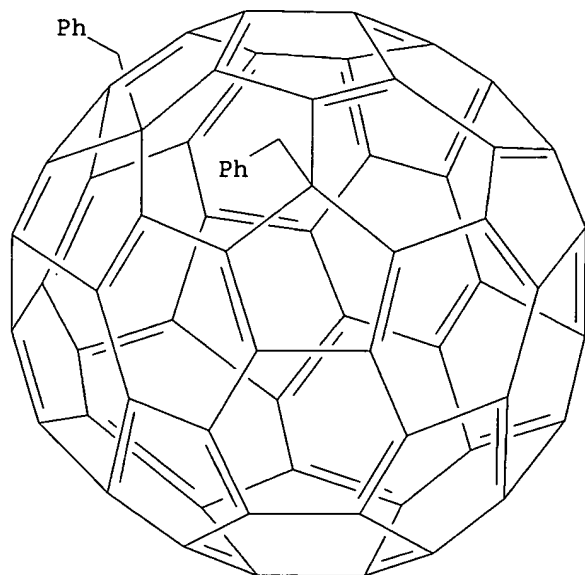
AB The synthesis, electrochem. and spectroscopic characterization of  
(C6H5CH2)4C60 is reported. A mechanism for the synthesis starting from  
(C6H5CH2)2C60 is proposed and involves an initial electron transfer  
between [(C6H5CH2)2C60]2- and C6H5CH2Br followed by a radical coupling  
process. Mass spectra and 1H NMR data indicate that several isomers of  
(C6H5CH2)4C60 are generated during the reaction and two of these are  
characterized in this paper as possessing C1 symmetry with the four benzyl  
groups being close to each other. Near IR spectra for one of the isomers  
of [(C6H5CH2)4C60]- and [(C6H5CH2)4C60]2- are reported and compared with  
spectra for mono- and dianionic C60 and (C6H5CH2)2C60. Electrochem. data  
are also reported for one of the two isolated (C6H5CH2)4C60 isomers.

IT 176106-61-9

RL: RCT (Reactant); RACT (Reactant or reagent)  
(benzylation of dibenzylfullerene)

RN 176106-61-9 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-dihydro-1,7-bis(phenylmethyl)- (9CI) (CA INDEX  
NAME)

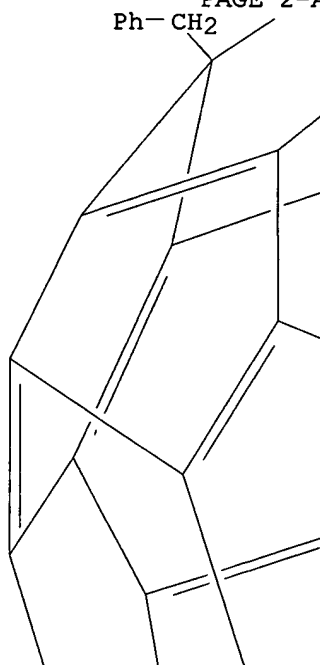


IT 207684-64-8 208119-55-5 208119-56-6  
 208119-58-8 208119-60-2 208119-62-4  
 RL: PRP (Properties)  
 (heat of formation of)  
 RN 207684-64-8 CAPLUS  
 CN [5,6]Fullerene-C60-Ih, 1,6,11,18-tetrahydro-1,6,11,18-  
 tetrakis(phenylmethyl)- (9CI) (CA INDEX NAME)

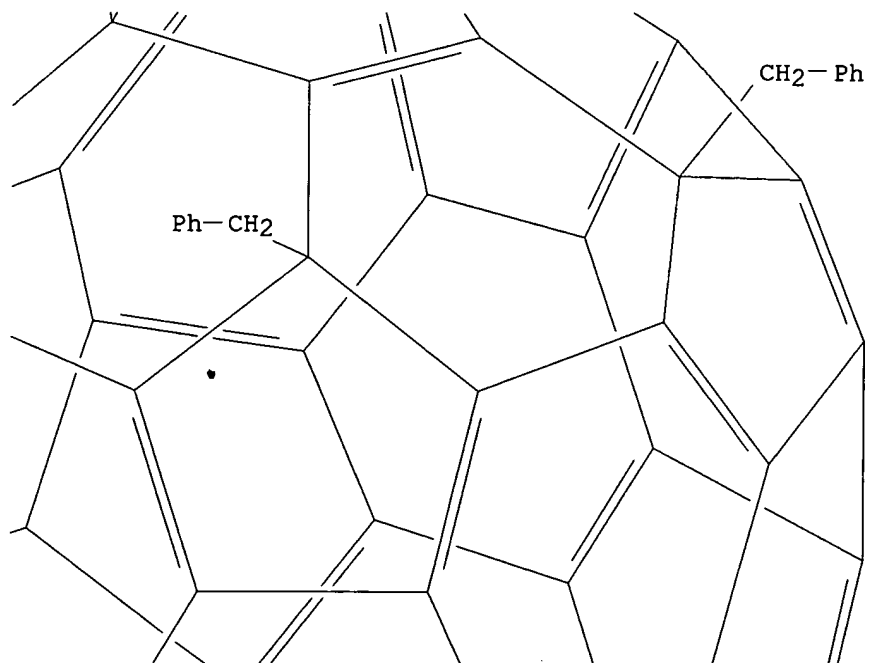
PAGE 1-A



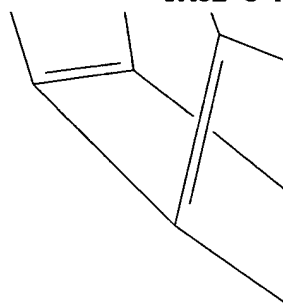
PAGE 2-A  
Ph-CH<sub>2</sub>



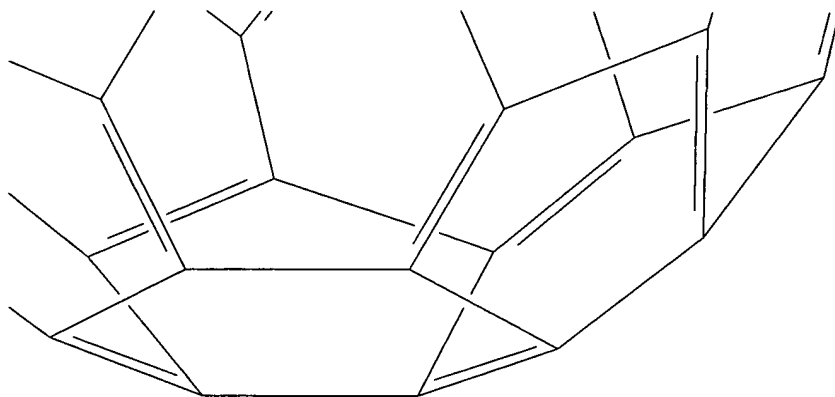
PAGE 2-B



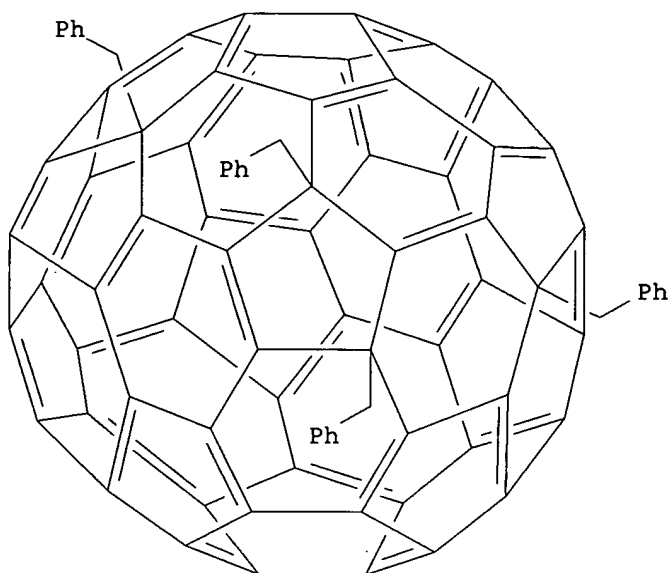
PAGE 3-A



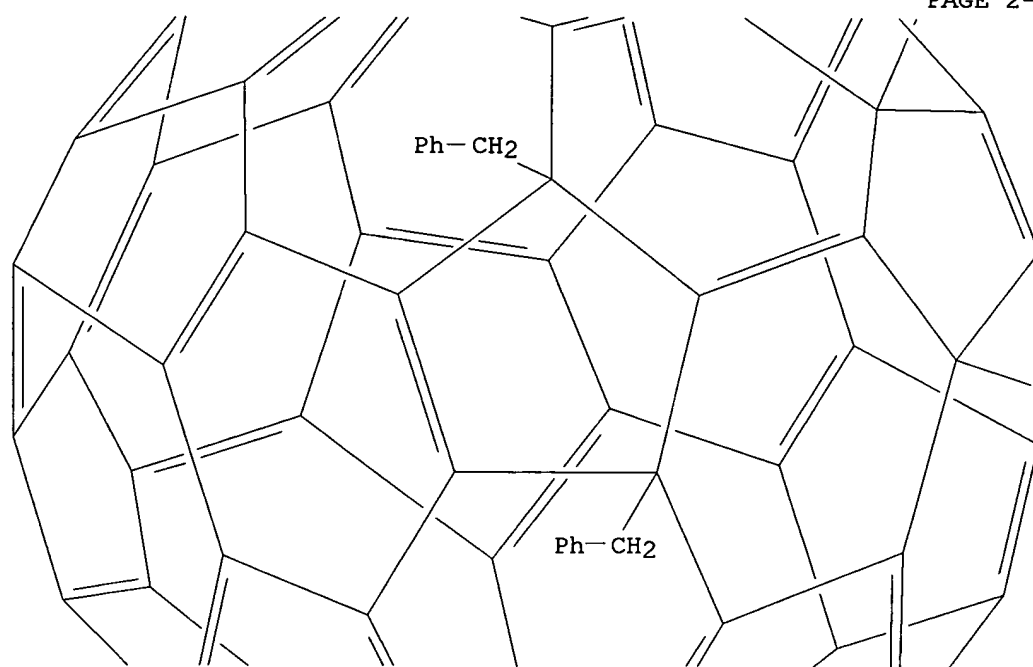
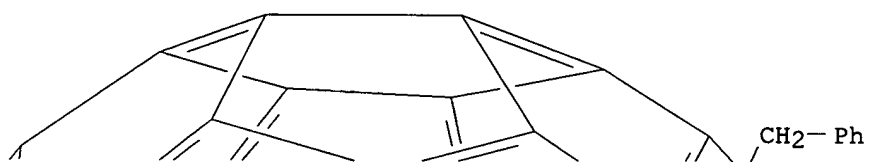




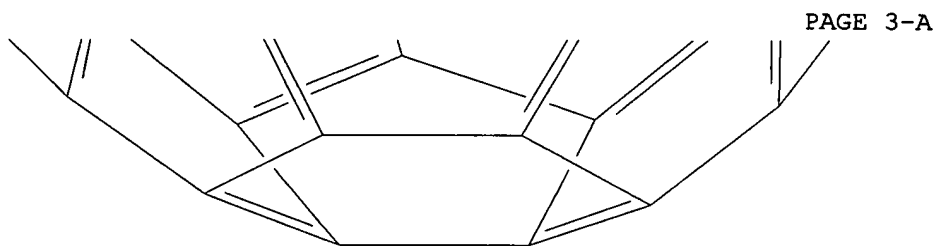
RN 208119-55-5 CAPLUS  
 CN [5,6]Fullerene-C60-Ih, 1,3,7,13-tetrakis(phenylmethyl)- (9CI) (CA INDEX NAME)



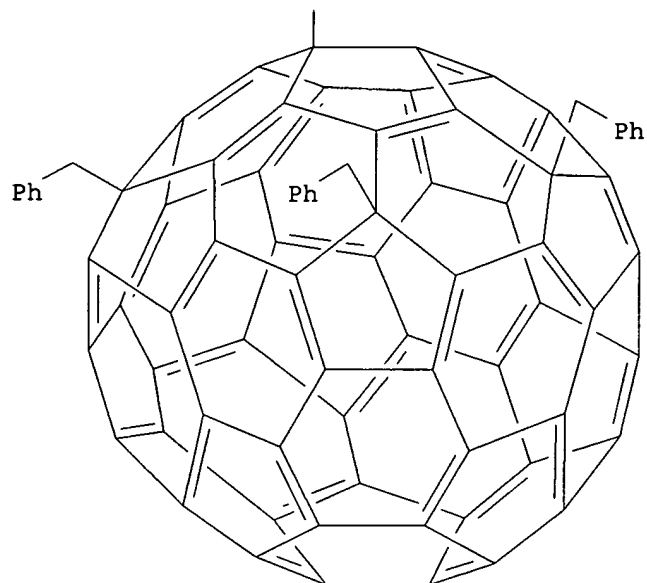
RN 208119-56-6 CAPLUS  
 CN [5,6]Fullerene-C60-Ih, 1,3,11,13-tetrakis(phenylmethyl)- (9CI) (CA INDEX NAME)



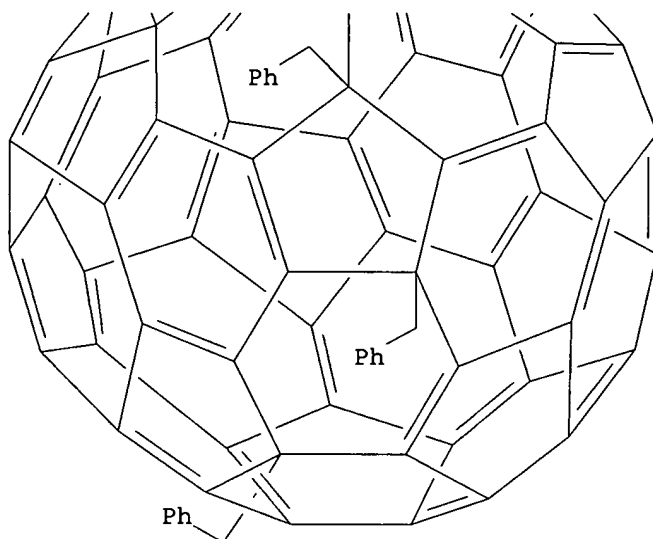
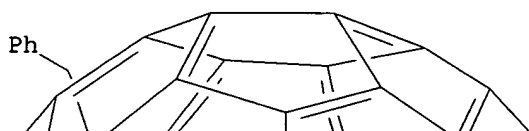
—CH<sub>2</sub>—Ph



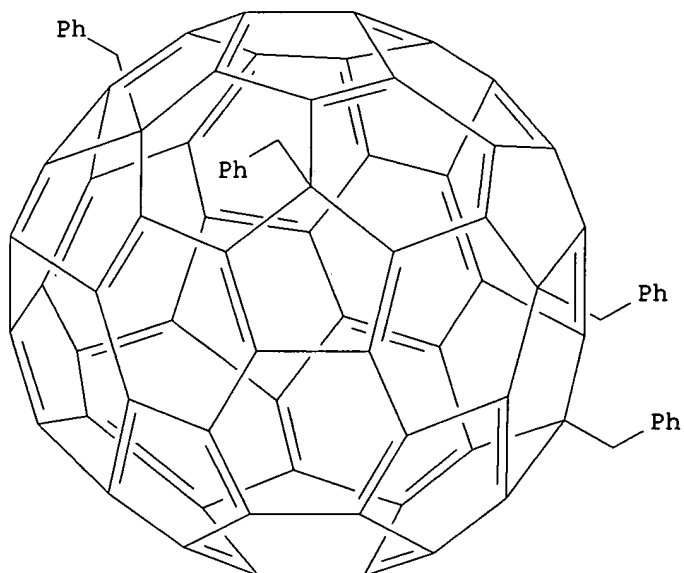
RN 208119-58-8 CAPLUS  
 CN [5,6]Fullerene-C60-Ih, 1,7,15,18-tetrakis(phenylmethyl)- (9CI) (CA INDEX  
 NAME)



RN 208119-60-2 CAPLUS  
 CN [5,6]Fullerene-C60-Ih, 1,3,7,17-tetrakis(phenylmethyl)- (9CI) (CA INDEX  
 NAME)



RN 208119-62-4 CAPLUS  
 CN [5,6]Fullerene-C60-Ih, 1,7,13,32-tetrakis(phenylmethyl)- (9CI) (CA INDEX  
 NAME)

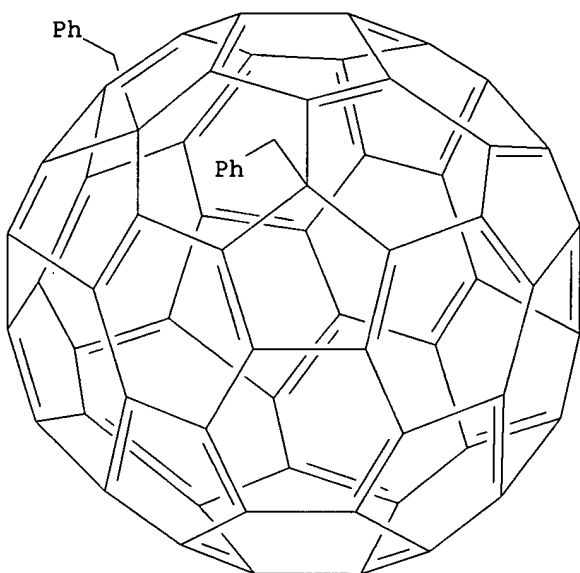


IT 182212-26-6

RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)  
(kinetics of reactions of dibenzylfullerene dianion and related compds. with alkyl halides)

RN 182212-26-6 CAPLUS

CN [5,6]Fullerene-C<sub>60</sub>-1h, 1,7-dihydro-1,7-bis(phenylmethyl)-, radical ion(2-)  
(9CI) (CA INDEX NAME)

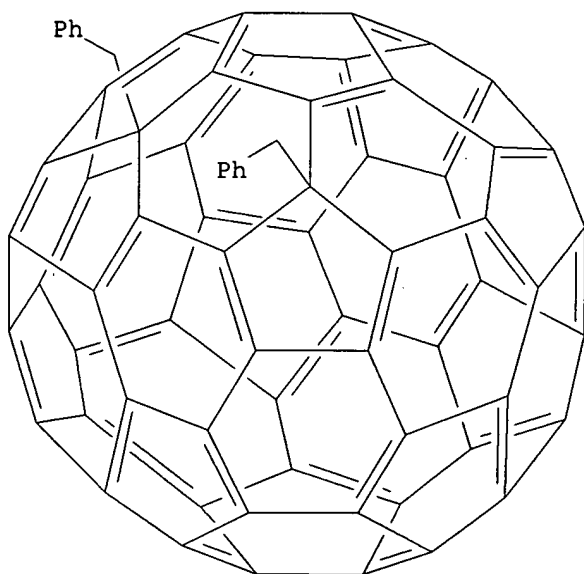


IT 182212-24-4

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(near IR spectra of)

RN 182212-24-4 CAPLUS

CN [5,6]Fullerene-C60-1h, 1,7-dihydro-1,7-bis(phenylmethyl)-, radical ion(1-)  
(9CI) (CA INDEX NAME)

RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 13 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1997:780509 CAPLUS

DN 128:173507

TI Photophysical investigation on molecular aggregation of  
1-benzyl-2-hydro[60]fullerene in Langmuir-Blodgett multilayersAU Ma, Shihong; Lu, Xingze; Xu, Jianhua; Zhou, Guangpeng; Cai, Zhigang; Zhou,  
Jianying; Wang, Wencheng; Li, YufenCS Department of Physics, Ion and Electron Beams, State Key Joint Laboratory  
for Materials Modification by Laser, Fudan University, Shanghai 200433,  
Peop. Rep. China

SO Chemical Physics Letters (1997), 280(3,4), 308-314

CODEN: CHPLBC; ISSN: 0009-2614

PB Elsevier Science B.V.

DT Journal

LA English

AB The aggregation behavior of a substituted fullerene compound,  
1-benzyl-2-hydro[60]fullerene (C60-Bh), in Z-type Langmuir-Blodgett (LB)  
multilayers was studied by UV-visible absorption, steady-state and  
time-resolved fluorescence spectroscopies. The LB multilayers of pure  
C60-Bh showed J-aggregate formation, characterized by a large red shift of  
2 absorption peaks ( $\Delta E$ .apprx.2098 cm<sup>-1</sup> from 260→275 nm and  
 $\Delta E$ .apprx.1076 cm<sup>-1</sup> from 328→340 nm). The main fluorescence  
emission bands were found at 710, 646, 603 and 595 nm for pure C60-Bh,  
mixed C60-Bh/arachidic acid (AA) (1:1), mixed C60-Bh/nitrogencrown (NC)  
(1:3) multilayers and monomeric C60-Bh in solution, resp. The aggregates  
were dissociated by mixing with AA or NC. The fluorescence decay profiles of  
C60-Bh, C60-Bh/AA and C60-Bh/NC in LB films could be fitted by a

bi-exponential decay model.

IT 170646-75-0 202921-96-8 202921-98-0

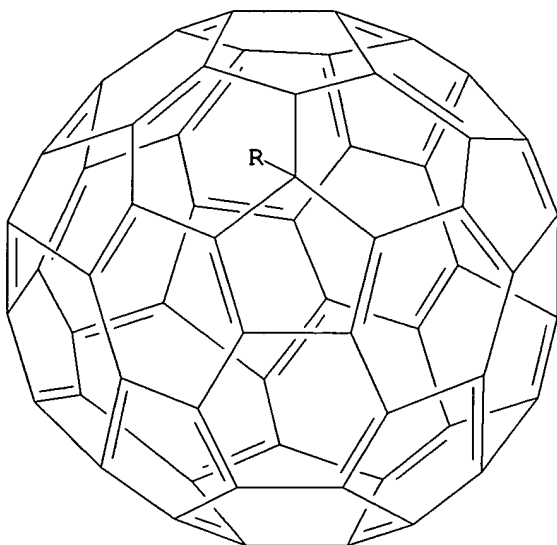
RL: PRP (Properties)

(mol. aggregation in Langmuir-Blodgett multilayers of)

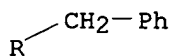
RN 170646-75-0 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,9-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



RN 202921-96-8 CAPLUS

CN Eicosanoic acid, compd. with 1,9-dihydro-1-(phenylmethyl)[5,6]fullerene-C60-Ih (1:1) (9CI) (CA INDEX NAME)

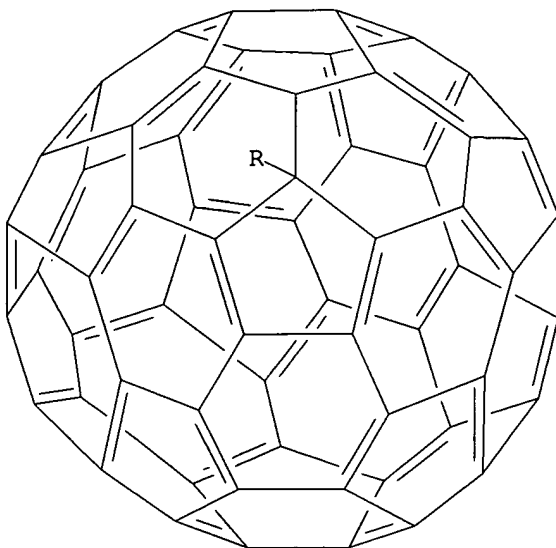
CM 1

CRN 170646-75-0

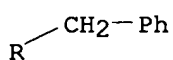
CMF C67 H8



PAGE 1-A



PAGE 2-A



CM 2

CRN 506-30-9

CMF C20 H40 O2

HO<sub>2</sub>C- (CH<sub>2</sub>)<sub>18</sub>-Me

RN 202921-98-0 CAPLUS

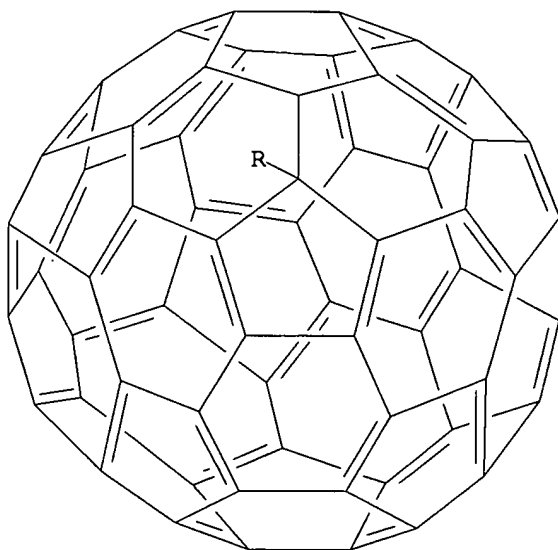
CN 1,4,7,10,13,16-Hexaazacyclooctadeca-1,3,10,12-tetraene,  
7,16-bis(1-oxooctadecyl)-, compd. with 1,9-dihydro-1-  
(phenylmethyl)[5,6]fullerene-C<sub>60</sub>-1h (3:1) (9CI) (CA INDEX NAME)

CM 1

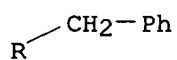
CRN 170646-75-0

CMF C67 H8

PAGE 1-A



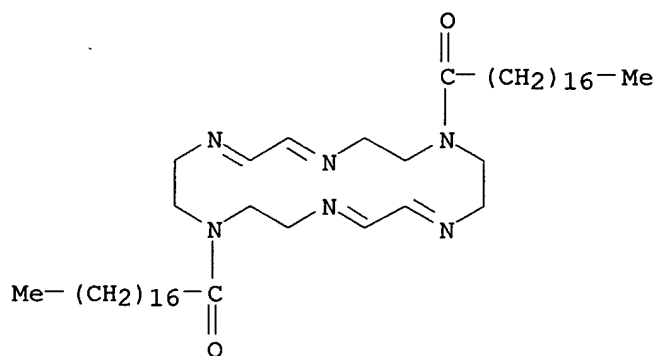
PAGE 2-A



CM 2

CRN 142706-29-4

CMF C48 H90 N6 O2



L5 ANSWER 14 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN

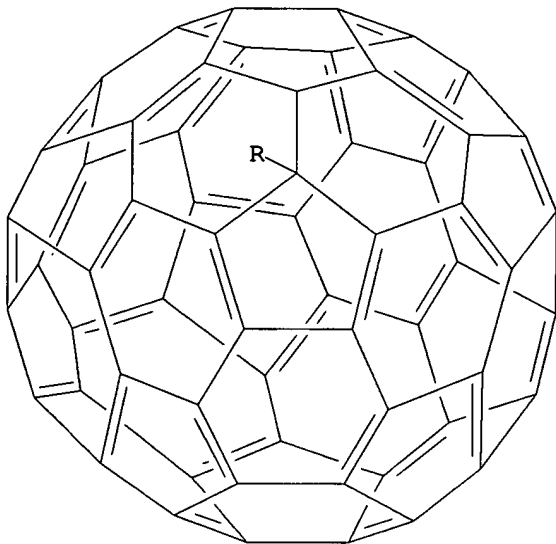
AN 1997:556509 CAPLUS

DN 127:176128

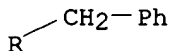
TI Quantum chemical studies on the structure and spectra of the addition product HC60CH2C6H5

AU Chen, Zhong-Fang; Teng, Qi-Wen; Wu, Shi; Pan, Yin-Ming; Zhao, Xue-Zhuang;  
Tang, Au-Chin; Feng, Ji-Kang  
CS Dep. Chem., Nankai Univ., Tianjin, 300071, Peop. Rep. China  
SO Gaodeng Xuexiao Huaxue Xuebao (1997), 18(8), 1346-1349  
CODEN: KTHPDM; ISSN: 0251-0790  
PB Gaodeng Jiaoyu Chubanshe  
DT Journal  
LA Chinese  
AB The INDO series methods have been used to study the structures for the two  
is kinds of isomers, which are 1,2-addition and 1,4-addition of HC60CH2C6H5. It  
is indicated that 1,2-HC60CG2C6H5 has Cs symmetry, while 1,4-HC60CH2C6H5 has  
no symmetry. Furthermore, the total energy of 1,2-isomer is higher than  
that of 1,4-isomer. The electronic spectra for both isomers have been  
calculated based on the optimized geometries and the reason for the red-shift  
of the spectra has been discussed.  
IT **170646-75-0 194145-24-9**  
RL: PRP (Properties)  
(MO calcn. of structure and UV of addition product HC60CH2C6H5)  
RN 170646-75-0 CAPLUS  
CN [5,6]Fullerene-C60-1h, 1,9-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX  
NAME)

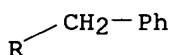
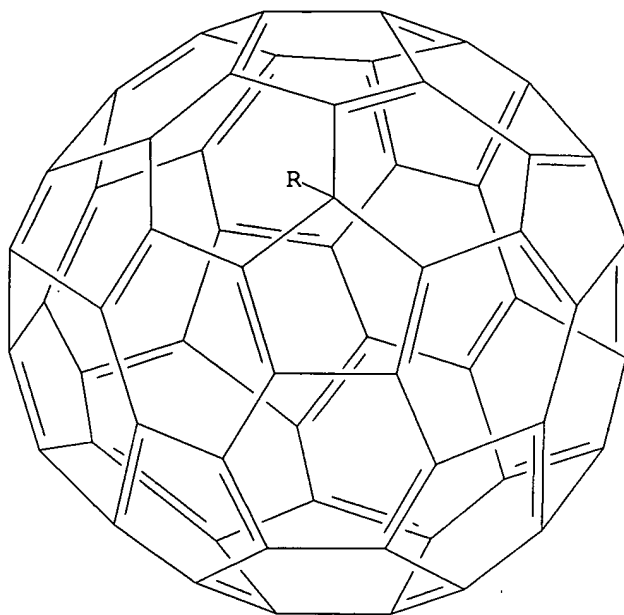
PAGE 1-A



PAGE 2-A



RN 194145-24-9 CAPLUS  
CN [5,6]Fullerene-C60-1h, 1,7-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX  
NAME)



- L5 ANSWER 15 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1997:551237 CAPLUS  
 DN 127:247723  
 TI Photoreactions with fullerenes  
 AU Mattay, Jochen; Siedschlag, Christina; Torres-Garcia, Gregorio; Ulmer, Lars; Wolff, Christian; Fujitsuka, Mamoru; Watanabe, Akira; Ito, Osamu; Luftmann, Heinrich  
 CS Institut fur Organische Chemie, Universitat Kiel, Kiel, D-24098, Germany  
 SO Proceedings - Electrochemical Society (1997), 97-14 (Recent Advances in the Chemistry and Physics of Fullerenes and Related Materials), 326-337  
 CODEN: PESODO; ISSN: 0161-6374  
 PB Electrochemical Society  
 DT Journal; General Review  
 LA English  
 AB The synthesis of azafulleroids and aziridinofullerenes is reported. Generally azafulleroids are formed upon thermolysis from azides. The corresponding aziridinofullerenes are obtained from the azafulleroids by irradiation, probably via a di- $\pi$ -methane rearrangement. Surprisingly [70]fullerene gives only two isomeric azafulleroids with Cs-symmetry. The photoreactions of 4-methyl-1,2,4-triazoline-3,5-dione (NMTAD) with various [60]fullerene derivs. have been studied. In general, [60]fullerenes with a closed structure cycloadd in a [2+2] fashion to NMTAD whereas 1,6-methano-[60]fulleroid undergoes a [2+2+2] cycloaddn. also in the

absence of light. Finally new preparative results and some preliminary time-resolved laser flash photolysis studies on the generation and the reactions of [60]fullerene radical cations are reported; 27 refs.

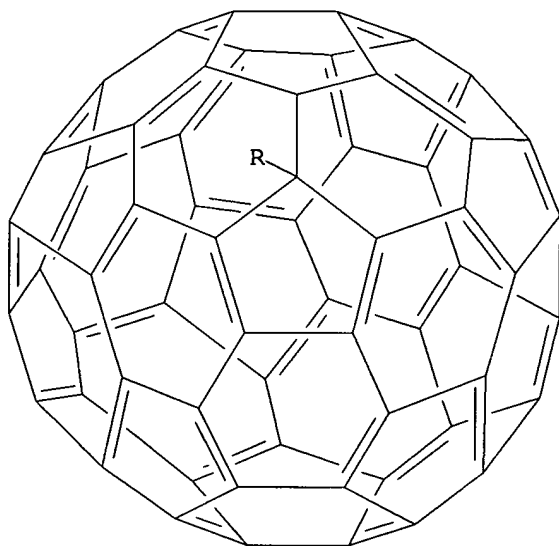
IT 170646-75-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(photochem. functionalization of C60)

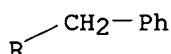
RN 170646-75-0 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,9-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 16 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1997:551224 CAPLUS

DN 127:247828

TI Electrogeneration, electrochemistry and spectroelectrochemistry of C60 adducts

AU Kadish, Karl M.; Gao, Xiang; Van Caemelbecke, Eric; Hirasaka, Takeomi; Suenobu, Tomoyoshi; Fukuzumi, Shunichi

CS Department of Chemistry, University of Houston, Houston, TX, 77204-5641, USA

SO Proceedings - Electrochemical Society (1997), 97-14 (Recent Advances in the Chemistry and Physics of Fullerenes and Related Materials), 221-235

CODEN: PESODO; ISSN: 0161-6374

PB Electrochemical Society

DT Journal

LA English

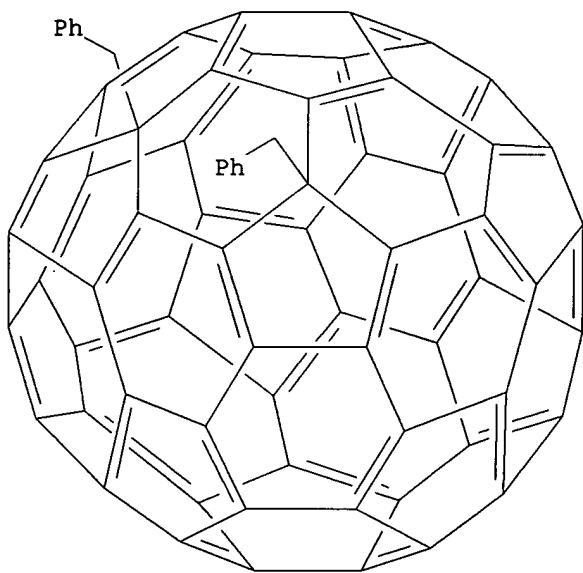
AB The synthesis, electrochem. and spectral characterization of fullerene derivs. of the type  $C_{60}(R)_2$ , where  $R = C_6H_5CH_2$ ,  $2-BrC_6H_4CH_2$ ,  $3-BrC_6H_4CH_2$  or  $4-BrC_6H_4CH_2$  is reported. Near-IR absorptions for both monoanions and dianions of the investigated compds. are blue- and red-shifted with respect to the near-IR absorptions of  $C_{60}^-$  and  $C_{60}^{2-}$ , resp.  $C_{60}(C_6H_5CH_2)_4$  was also electro-synthesized and characterized by mass spectrometry,  $^1H$  NMR,  $^{13}C$  NMR, UV-visible spectroscopy and electrochem. The isolated compound has a  $C_1$  symmetry and a possible structure is discussed on the basis of NMR and UV-visible data.

IT **182212-24-4P 182212-26-6P 195625-44-6P**  
**195625-45-7P 195625-46-8P 195738-81-9P**  
**195738-82-0P 195738-83-1P**

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (near IR spectra of  $C_{60}$  adduct anions)

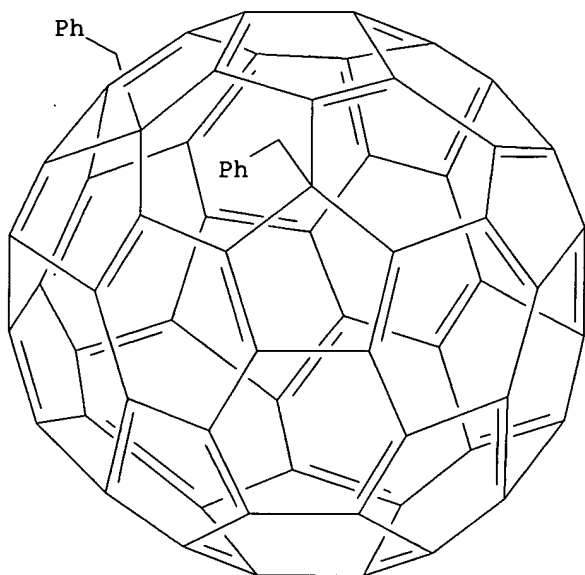
RN 182212-24-4 CAPLUS

CN [5,6]Fullerene- $C_{60}$ -Ih, 1,7-dihydro-1,7-bis(phenylmethyl)-, radical ion(1-)  
 (9CI) (CA INDEX NAME)



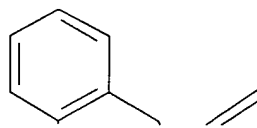
RN 182212-26-6 CAPLUS

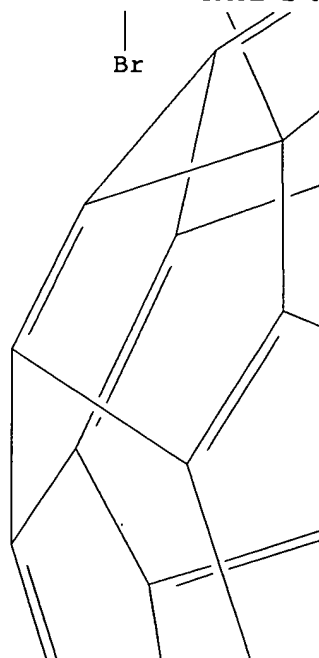
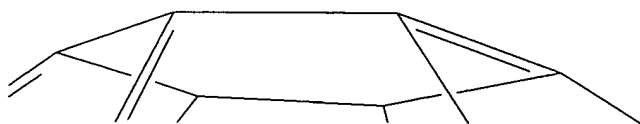
CN [5,6]Fullerene- $C_{60}$ -Ih, 1,7-dihydro-1,7-bis(phenylmethyl)-, radical ion(2-)  
 (9CI) (CA INDEX NAME)



RN 195625-44-6 CAPLUS  
 CN [5,6]Fullerene-C60-1h, 1,7-bis[(2-bromophenyl)methyl]-1,7-dihydro-,  
 radical ion(1-) (9CI) . (CA INDEX NAME)

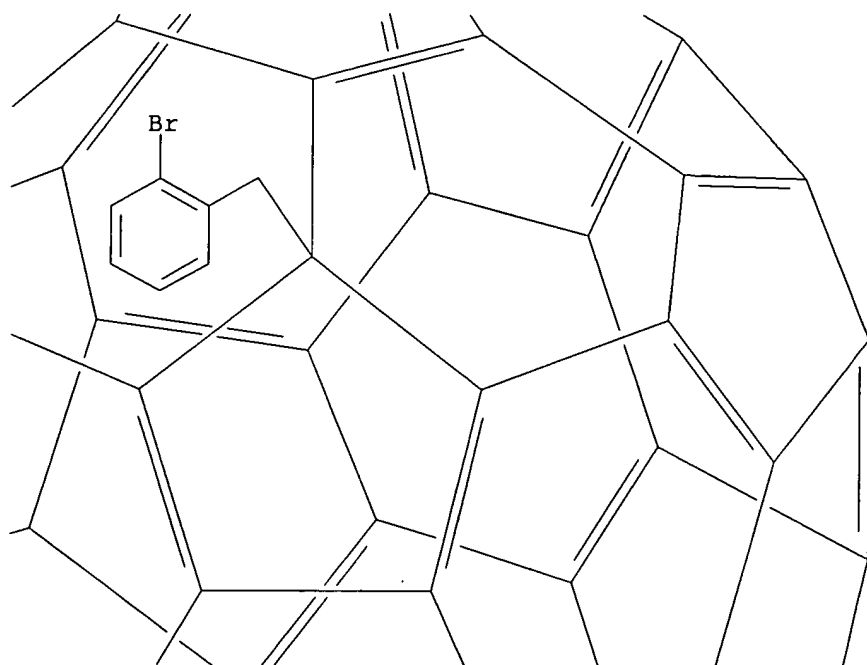
PAGE 1-A



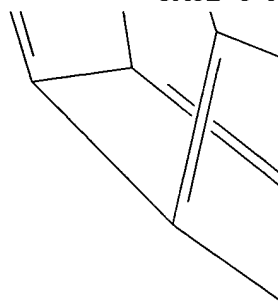




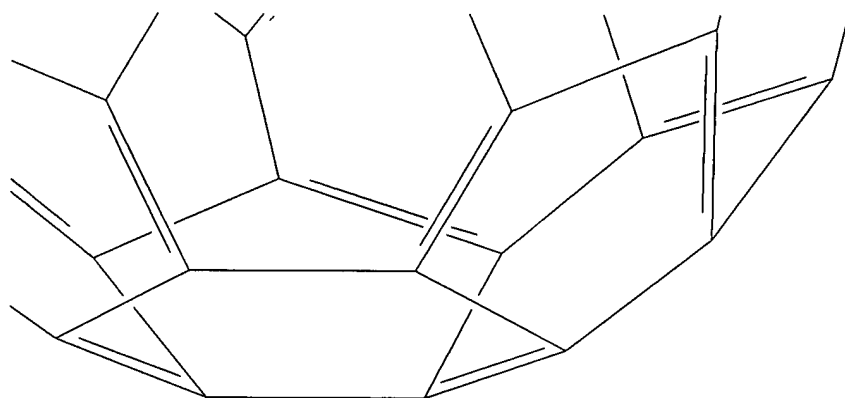
PAGE 2-B



PAGE 3-A



PAGE 3-B



RN 195625-45-7 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-bis[(3-bromophenyl)methyl]-1,7-dihydro-,  
radical ion(1-) (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 195625-46-8 CAPLUS

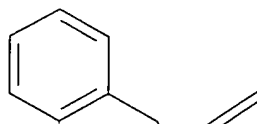
CN [5,6]Fullerene-C60-Ih, 1,7-bis[(4-bromophenyl)methyl]-1,7-dihydro-,  
radical ion(1-) (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

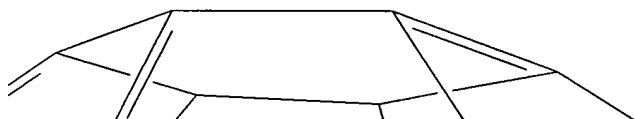
RN 195738-81-9 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-bis[(2-bromophenyl)methyl]-1,7-dihydro-,  
radical ion(2-) (9CI) (CA INDEX NAME)

PAGE 1-A

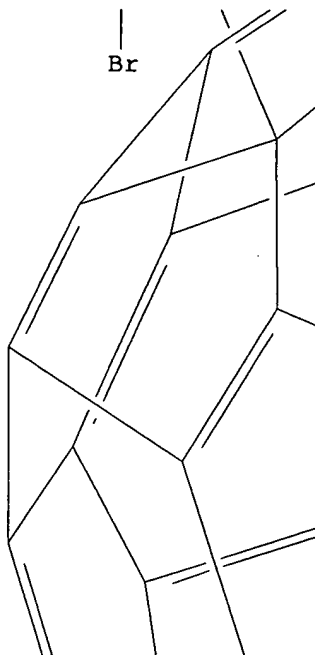


PAGE 1-B

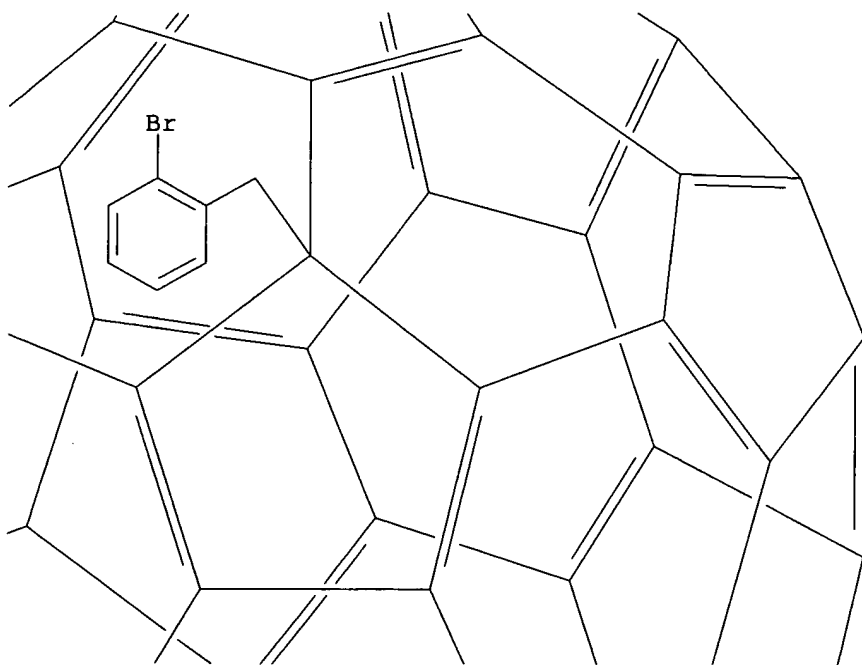


PAGE 2-A

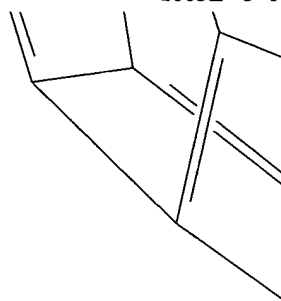
Br

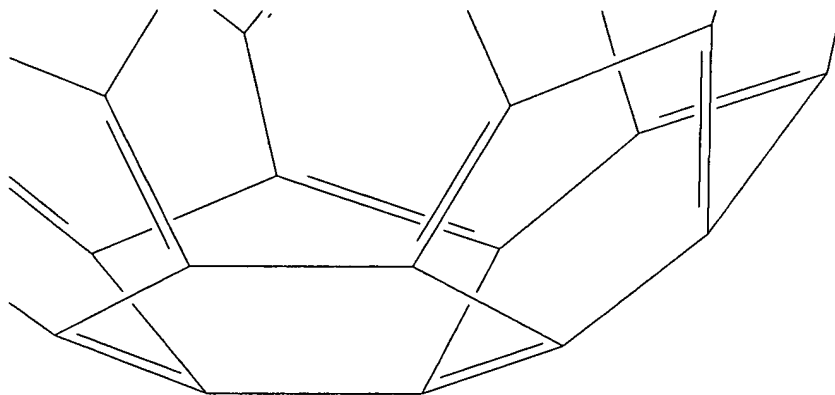


PAGE 2-B



PAGE 3-A





RN 195738-82-0 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-bis[(3-bromophenyl)methyl]-1,7-dihydro-,  
radical ion(2-) (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 195738-83-1 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-bis[(4-bromophenyl)methyl]-1,7-dihydro-,  
radical ion(2-) (9CI) (CA INDEX NAME)

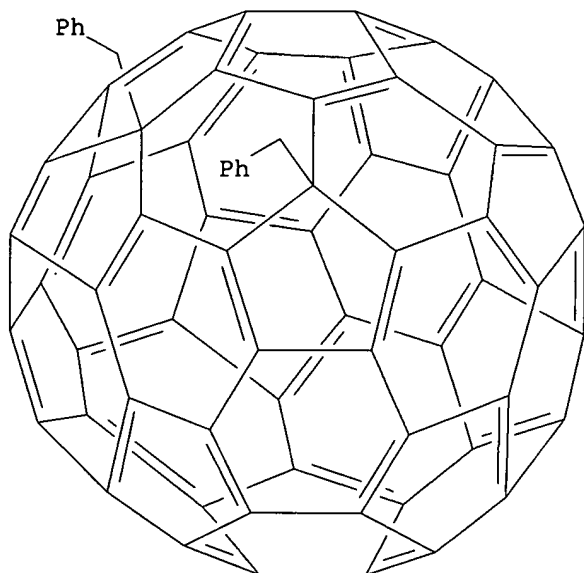
\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

IT **176106-61-9P 195625-41-3P 195625-42-4P**  
**195625-43-5P**

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT  
(Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC  
(Process); RACT (Reactant or reagent)  
(synthesis, electrochem. and spectral characterization of fullerene  
derivs)

RN 176106-61-9 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-dihydro-1,7-bis(phenylmethyl)- (9CI) (CA INDEX  
NAME)



RN 195625-41-3 CAPLUS  
 CN [5,6]Fullerene-C60-1h, 1,7-bis[(2-bromophenyl)methyl]-1,7-dihydro- (9CI)  
 (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 195625-42-4 CAPLUS  
 CN [5,6]Fullerene-C60-1h, 1,7-bis[(3-bromophenyl)methyl]-1,7-dihydro- (9CI)  
 (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RN 195625-43-5 CAPLUS  
 CN [5,6]Fullerene-C60-1h, 1,7-bis[(4-bromophenyl)methyl]-1,7-dihydro- (9CI)  
 (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 17 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1997:551220 CAPLUS  
 DN 127:234001  
 TI Generation of C60 adducts with two different alkyl groups in the reactions  
 between C2-60 and alkyl halides  
 AU Fukuzumi, Shunichi; Suenobu, Tomoyoshi; Hirasaka, Takeomi; Gao, Xiang; Van  
 Caemelbecke, Eric; Kadish, Karl M.  
 CS Department of Applied Chemistry, Faculty of Engineering, Osaka University,  
 Suita, 565, Japan  
 SO Proceedings - Electrochemical Society (1997), 97-14(Recent  
 Advances in the Chemistry and Physics of Fullerenes and Related  
 Materials), 173-185  
 CODEN: PESODO; ISSN: 0161-6374  
 PB Electrochemical Society  
 DT Journal  
 LA English  
 AB Symposium proceedings. The C602- generated in the reduction of C60 with

naphthalene radical anion in benzonitrile reacts with various alkyl halides (RX) to yield the corresponding mono-alkyl adduct anions RC60-. An extensive comparison of the rate consts. for the alkylation of C2-60 with RX with those of electron transfer from tetramethylseminquinone radical anion to the same series of RX demonstrates clearly that electron transfer from C2-60 to RX is the rate-determining step in the alkylation of C602-. A mono-alkyl adduct anion, t-BuC60-, produced in the reaction of C602- with t-BuI undergoes no further reaction with t-BuI, but the SN2 reaction proceeds with less sterically hindered RX to produce dialkyl-substituted C60 with different alkyl groups, i.e., (t-Bu)(C6H5CH2)C60. Protonation of t-BuC60- with trifluoroacetic acid occurs to produce (t-Bu)HC60. Extensive kinetic studies on the reactions of t-BuC60- with RX are compared with those for the authentic SN2 reactions of cobalt(I) tetraphenylporphyrin anion with RX and reveal that the reactions of t-BuC60- with RX proceed via a SN2 pathway rather than an electron transfer pathway. The difference in reactivities between the electron transfer and SN2 reactions enable us to prepare dialkyl-substituted C60 with two different alkyl groups.

IT 182070-59-3

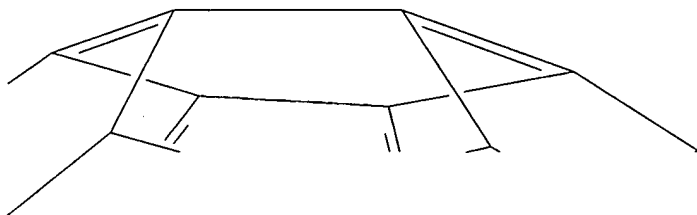
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(kinetics and mechanism of 2-step alkylation of fullerene dianion with alkyl halides)

RN 182070-59-3 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,2-dihydro-1-(phenylmethyl)-, ion(1-) (9CI) (CA INDEX NAME)

PAGE 1-A



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

IT **195392-52-0**

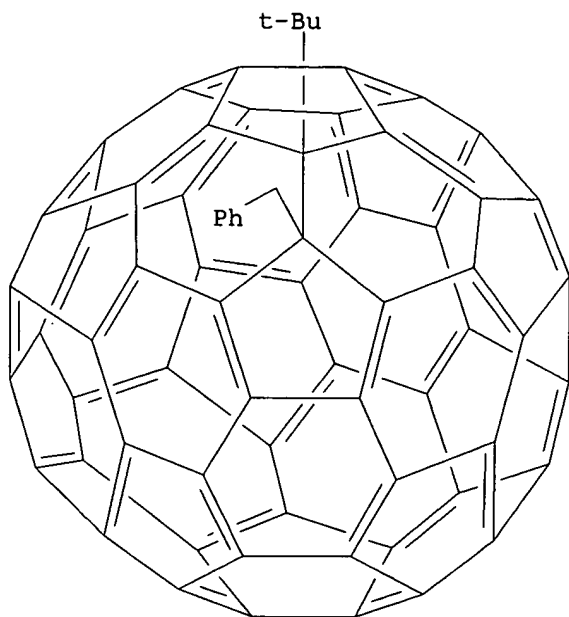
RL: PRP (Properties)

(kinetics and mechanism of 2-step alkylation of fullerene dianion with alkyl halides)

RN 195392-52-0 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1-(1,1-dimethylethyl)-1,9-dihydro-9-(phenylmethyl)-(9CI) (CA INDEX NAME)





IT **160482-48-4P**

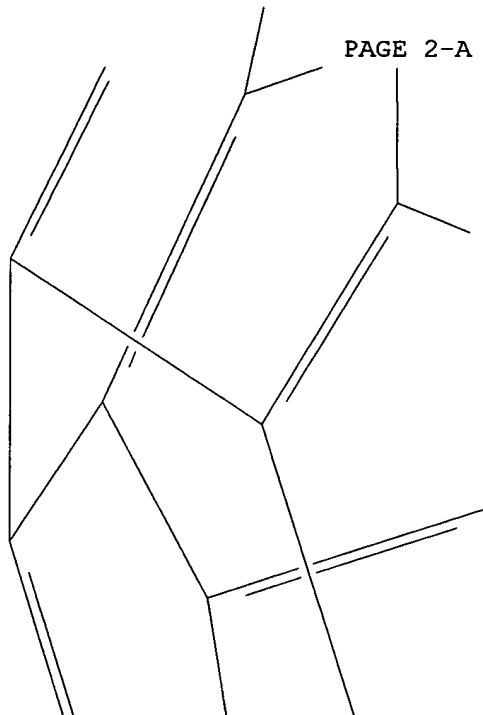
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(kinetics and mechanism of 2-step alkylation of fullerene dianion with  
alkyl halides)

RN 160482-48-4 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1-(1,1-dimethylethyl)-1,7-dihydro-7-(phenylmethyl)-  
(9CI) (CA INDEX NAME)

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

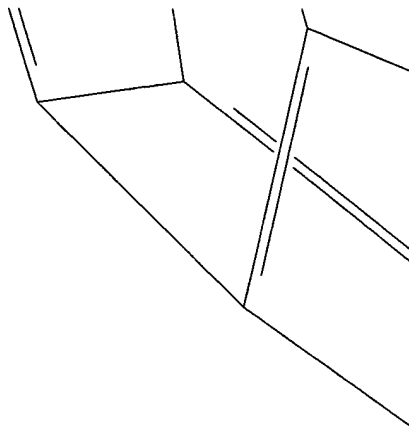
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*



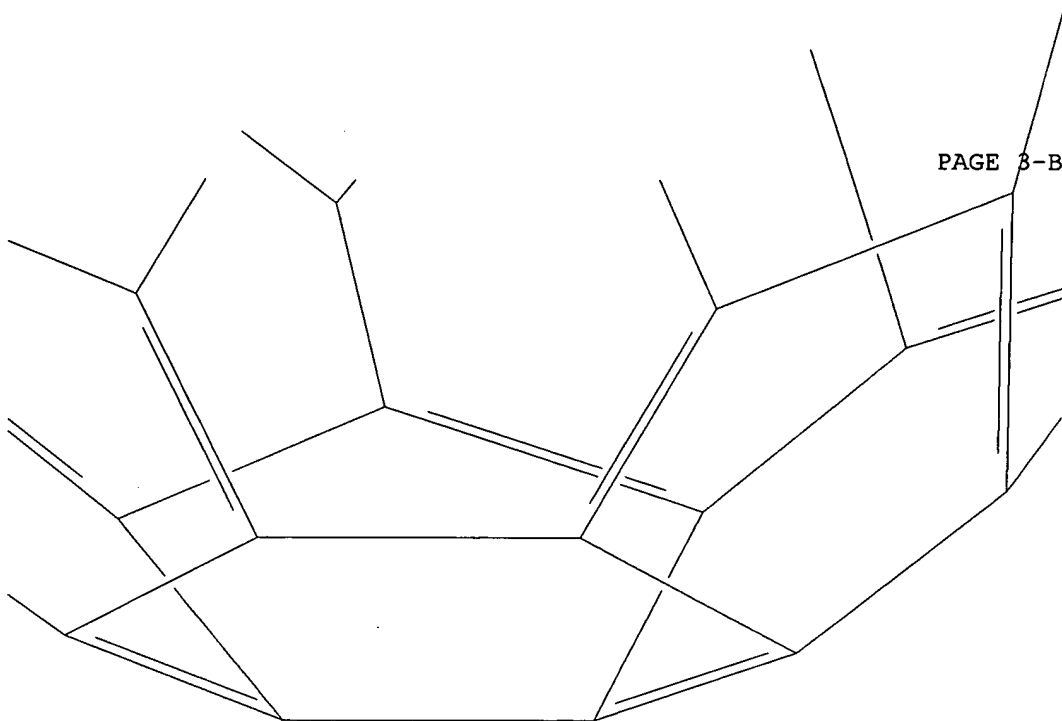
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

PAGE 3-A



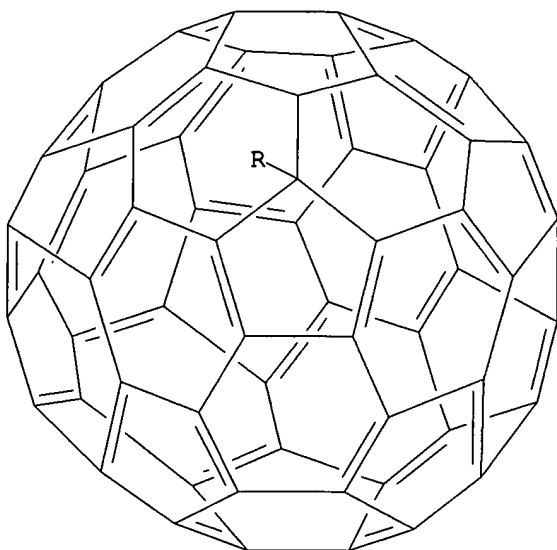
PAGE 3-B



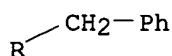
RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 18 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1997:523807 CAPLUS  
DN 127:240547  
TI Fabrication and optical nonlinearities of Langmuir-Blodgett multilayers of  
1-benzyl-9-hydrofullerene-60  
AU Ma, Shihong; Lu, Xingze; Han, Kui; Liu, Liying; Wang, Gongming; Wang,  
Wencheng; Li, Yufen; Chen, Jian; Cai, Ruifang; Huang, Zu'en  
CS Dep. Phys., Fudan Univ., Shanghai, 200433, Peop. Rep. China  
SO Guangxue Xuebao (1996), 16(11), 1600-1606  
CODEN: GUXUDC; ISSN: 0253-2239  
PB Kexue  
DT Journal  
LA Chinese  
AB The structural features of the Langmuir-Blodgett (LB) films of substituted  
fullerene C60-Be was studied by  $\pi$ -A isotherm, small angle x-ray  
diffraction (SAXD), and optical measurements. Pure C60-Br mols. at the  
air-H2O interface in a bulk phase were found. 1,10-Bis(stearyl)-4,6,13,15-  
tetraene-18-nitrogencrown-6 (NC) was used as an inert material to  
construct mixed C60-Be/NC LB films which had a much better quality than  
the pure C60-Be LB films. The structural improvement in the mixed  
C60-B/NC LB films was realized by  $\pi$ -A isotherm, UV-visible absorption,  
and SAXD measurements as an insertion of C60-Be mols. between the two  
chains of NC. The 3rd-order nonlinear susceptibility XXXXX(3) is  
 $(-3\omega; \omega, \omega, \omega) = 2.1 + 10^{-11}$  esu by the method  
of three-harmonic generation in mixed C60-Be/NC LB films.  
IT **170646-75-0**  
RL: PRP (Properties)  
(fabrication and optical nonlinearities of Langmuir-Blodgett  
multilayers of 1-benzyl-9-hydrofullerene-60 with crown derivative)  
RN 170646-75-0 CAPLUS  
CN [5,6]Fullerene-C60-Ih, 1,9-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX  
NAME)

PAGE 1-A



PAGE 2-A



L5 ANSWER 19 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1997:479924 CAPLUS  
 DN 127:240782  
 TI Enhanced coalescence reactions of fullerenes by laser desorption of C60 derivatives  
 AU Ong, P. P.; Zhu, Lei; Zhao, Li; Zhang, Jun; Wang, Shenyi; Li, Yufen; Cai, Ruifang; Huang, Zuen  
 CS Dep. of Phys., Natl. Univ. of Singapore, Singapore, 0511, Singapore  
 SO International Journal of Mass Spectrometry and Ion Processes (1997), 163(1,2), 19-28  
 CODEN: IJMPDN; ISSN: 0168-1176  
 PB Elsevier  
 DT Journal  
 LA English  
 AB We observed enhanced coalescence reactions of fullerenes by laser desorption of chemical adducts of (C6HCH2)<sub>n</sub>C60, (C9H7)<sub>m</sub>HnC60, (CCl2)<sub>x</sub>C60 and the newly available poly-N-vinylcarbazole (PVK)-C60/70. The mass spectra of the laser-produced species reveal a characteristic bi-modal profile, with one maximum abundance distribution of parent fullerene ions located at C60 and the other at nearly twice C60. The mass spectra of both pristine C60 and the non-reactive PS/C60 mixture show monotonically descending intensity of daughter fullerenes with successive C2 captures, whereas slightly enhanced coalescence products are observed for the reactive PVK/C60/70 mixture which is known as a charge transfer complex. The mechanism of efficient coalescence is believed to be cluster collisional nucleation of pairs of reactive fullerene fragments (nascent C60, C58, etc.) induced by photofragmentation of the reactive R<sub>n</sub>-C60 adduct or

Rn...C60 charge transfer system, which is indicated by the laser power dependence features and the correlation between enhanced fullerene fragments and coalescence products.

IT **140656-83-3P**

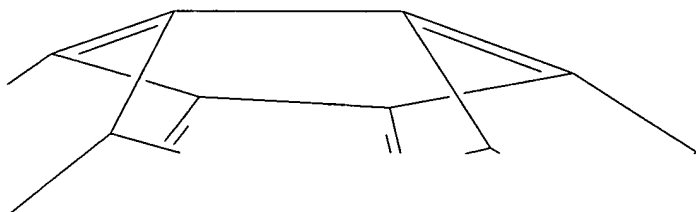
RL: ANT (Analyte); PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); PROC (Process)

(enhanced coalescence reactions of fullerenes by laser desorption of C60 derivs.)

RN 140656-83-3 CAPLUS

CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 2-(phenylmethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 20 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1997:110816 CAPLUS

DN 126:144421

TI Addition reaction of allylic stannanes to the triplet excited state of C60  
via photoinduced electron-transfer process leading to asymmetric  
hybridization chemistry for fullerene terpenoid

AU Mikami, Koichi; Matsumoto, Shoji; Tono, Takayuki; Suenobu, Tomoyoshi;  
Ishida, Akito; Fukuzumi, Shunichi

CS Dep. Chem. Technol., Tokyo Inst. Technol., Tokyo, 152, Japan

SO Synlett (1997), (1), 85-87

CODEN: SYNLES; ISSN: 0936-5214

PB Thieme

DT Journal

LA English

OS CASREACT 126:144421  
 AB Addition of allylic stannanes to C60 takes place under UV-irradiation in C6H6  
 or  
 PhCN to yield the allylic fullerenes. An enantiopure fullerene terpenoid  
 was obtained when a pinene-derived allylic stannane was used.

IT **186696-07-1P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of allylfullerenes by photoaddn. of allylic stannanes to C60)

RN 186696-07-1 CAPLUS  
 CN [5,6]Fullerene-C60-1h, 1-[(6,6-dimethylbicyclo[3.1.1]hept-2-en-2-yl)methyl]-1,9-dihydro-, (-)- (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

L5 ANSWER 21 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1996:677390 CAPLUS  
 DN 126:24514  
 TI Efficient optical nonlinear Langmuir-Blodgett films: Roles of matrix  
 molecules  
 AU Ma, Shihong; Lu, Xingze; Liu, Liying; Han, Kui; Wang, Wencheng; Zhang,  
 Zhiming  
 CS Department Physics, Fudan University, Shanghai, 200433, Peop. Rep. China  
 SO Proceedings of SPIE-The International Society for Optical Engineering (   
 1996), 2897(Electro-Optic and Second Harmonic Generation  
 Materials, Devices, and Applications), 59-67  
 CODEN: PSISDG; ISSN: 0277-786X  
 PB SPIE-The International Society for Optical Engineering  
 DT Journal  
 LA English

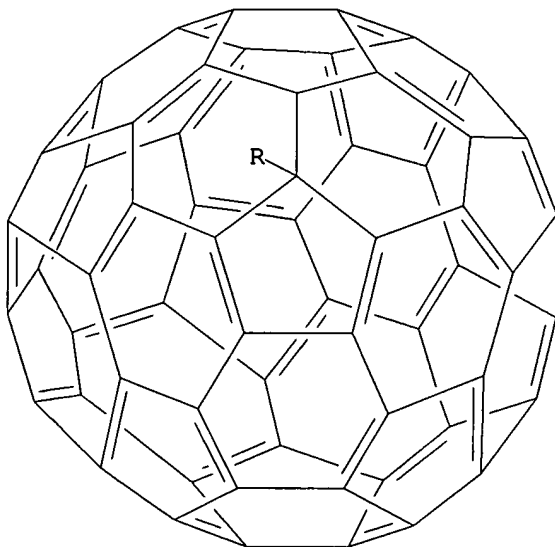
AB A novel bifat-chain amphiphilic mol. nitrogen-crown (NC) was adopted as an  
 inert material for fabrication of optical nonlinear Langmuir-Blodgett (LB)  
 multilayers. Structural improvement in the Z-type mixed fullerene derivative  
 (C60-Be)/NC LB multilayers samples was realized by insertion of the C60-Be  
 mols. between two hydrophobic chains of the NC mols. The relatively large  
 3rd-order susceptibility  $\chi(3)_{xxxx}(-3\omega; \omega, \omega, \omega) =$   
 $2.9 + 10^{-19} \text{ M}^2 \text{V}^2$  (or  $2.1 + 10^{-11} \text{ esu}$ ) was deduced by measuring  
 3rd harmonic generation (THG) from the C60-Be samples. The 2nd harmonic  
 generation (SHG) intensity increased quadratically with the bilayer number  
 (up to 116 bilayers) in Y-type hemicyanine (HEM)/NC interleaving LB  
 multilayers due to improvement of the structural properties by insertion  
 of the long hydrophobic tail of HEM mols. between two chains of NC mols.  
 The 2nd-order susceptibility  $\chi(2)_{zxx}(-2\omega; \omega, \omega) = 18$   
 $\text{pM V}^{-1}$  (or  $4.35 + 10^{-8} \text{ esu}$ ) was obtained by measuring SHG from the  
 HEM samples. The NC mol. has attractive features as a matrix material in  
 fabrications of LB multilayers made from optically nonlinear materials  
 with hydrophobic long tails or ball-like mols.

IT **170646-75-0**  
 RL: OCU (Occurrence, unclassified); PRP (Properties); OCCU (Occurrence)  
 (efficient optical nonlinear Langmuir-Blodgett films and their  
 properties and role of matrix mols.)

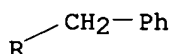
RN 170646-75-0 CAPLUS  
 CN [5,6]Fullerene-C60-1h, 1,9-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX  
 NAME)



PAGE 1-A



PAGE 2-A

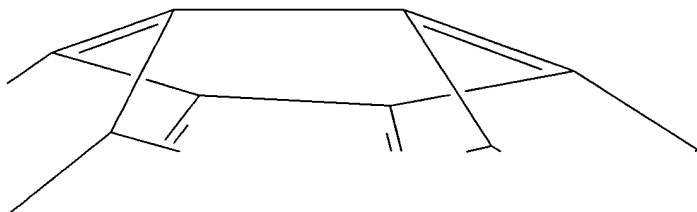


L5 ANSWER 22 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1996:570714 CAPLUS  
 DN 125:300590  
 TI Chemical generation of C60 anions and the alkylation with alkyl halides via electron transfer  
 AU Fukuzumi, Shunichi; Suenobu, Tomoyoshi; Kadish, K. M.; Subramanian, R.; Jones, M. T.  
 CS Dep. Appl. Chem., Osaka Univ., Osaka, 565, Japan  
 SO Proceedings - Electrochemical Society (1996), 96-10 (Recent Advances in the Chemistry and Physics of Fullerenes and Related Materials, Vol. 3), 243-252  
 CODEN: PESODO; ISSN: 0161-6374  
 PB Electrochemical Society  
 DT Journal  
 LA English  
 AB The naphthalene radical anion was used as an electron transfer reductant to reduce C60 to generate C60•<sup>-</sup>, C602<sup>-</sup>, and C60•3<sup>-</sup> in benzonitrile. The C602<sup>-</sup> thus generated reacts with various alkyl halides (RX) to yield the radical anions of the corresponding dialkyl derivs. R2C60•<sup>-</sup>. The R2C60 was obtained after the workup. The 2nd-order rate consts. of the alkylation of C602<sup>-</sup> with various alkyl halides are determined by monitoring the decrease in absorbance due to C602<sup>-</sup>. The reactivity of RX is rather insensitive to the steric hindrance of the alkyl groups of RX, being opposite from what is expected for the normal reactivity in the SN2 reaction. Such insensitiveness to the steric hindrance is shown to agree well with the reactivity of RX in the electron transfer reduction by a 1-electron reductant. An extensive comparison between the rate consts. of

the alkylation of C602- with various RX and those of electron transfer from tetramethylsemiquinone radical anion to the same series of RX demonstrates clearly that electron transfer from C602- to RX is the rate-determining step in the alkylation of C602-. A novel reaction mechanism of sequential electron transfer and SN2 is presented based on the kinetic studies on the alkylation of C602-, being specific to fullerene anions in which electrons are highly delocalized.

IT 182070-59-3  
RL: PRP (Properties)  
(PM3 calcn. of charge distribution in)  
RN 182070-59-3 CAPLUS  
CN [5,6]Fullerene-C60-Ih, 1,2-dihydro-1-(phenylmethyl)-, ion(1-) (9CI) (CA INDEX NAME)

PAGE 1-A



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

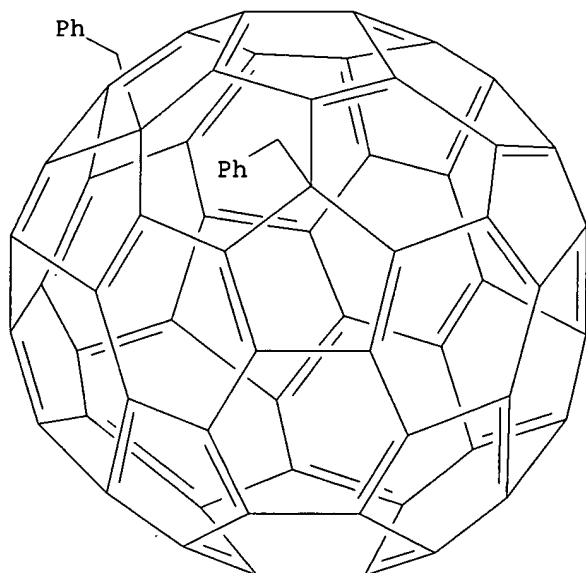
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

IT **176106-61-9P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 176106-61-9 CAPLUS

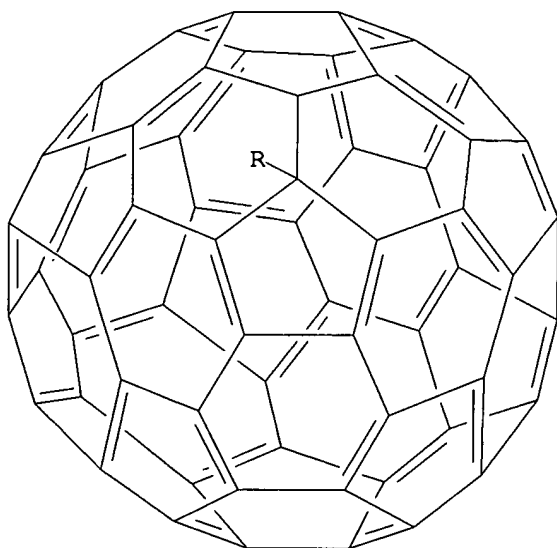
CN [5,6]Fullerene-C60-Ih, 1,7-dihydro-1,7-bis(phenylmethyl)- (9CI) (CA INDEX  
NAME)



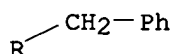
L5 ANSWER 23 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1996:569590 CAPLUS  
 DN 125:288019  
 TI Structural and Optical Nonlinear Characterizations of Langmuir-Blodgett  
 Films of 1-Benzyl-9-hydrofullerene-60  
 AU Ma, Shihong; Lu, Xingze; Chen, Jian; Han, Kui; Liu, Liying; Huang, Zuen;  
 Cai, Ruifang; Wang, Gongming; Wang, Wencheng; Li, Yufen  
 CS Department of Physics, Fudan University, Shanghai, 200433, Peop. Rep.  
 China  
 SO Journal of Physical Chemistry (1996), 100(41), 16629-16632  
 CODEN: JPCHAX; ISSN: 0022-3654  
 PB American Chemical Society  
 DT Journal  
 LA English  
 AB The structural and optical nonlinear features of the condensed layers at  
 the air-H<sub>2</sub>O interface and Langmuir-Blodgett (LB) films of the substituted  
 fullerene 1-benzyl-9-hydrofullerene-60 (C<sub>60</sub>-Be) were studied by  $\pi$ -A  
 isotherm, small angle x-ray diffraction (SAXD), and optical measurements.  
 Pure C<sub>60</sub>-Be mols. existed at the air-H<sub>2</sub>O interface in a bulk phase. A new  
 type of 2-chain amphiphilic mol., 1,10-bistearyl-4,6,13,15-tetraene-18-N-  
 crown-6 (NC), was used as an inert material to construct mixed C<sub>60</sub>-Be/NC  
 LB films of much better quality than the pure C<sub>60</sub>-Be LB films.  $\pi$ -A,  
 UV-visible spectra, and SAXD measurements show that the structural  
 improvement in the mixed C<sub>60</sub>-Be/NC LB films was realized by insertion of  
 the C<sub>60</sub>-Be mols. between the 2 hydrophobic chains of the NC mols. The  
 relatively large 3rd-order nonlinear susceptibility  $\chi(3)_{xxxx}(-3\omega;$   
 $\omega, \omega, \omega) = 2.1 \times 10^{-11}$  esu was deduced by measuring  
 3rd-harmonic generation in the mixed C<sub>60</sub>-Be/NC LB films.  
 IT **170646-75-0**, 1-Benzyl-9-hydrofullerene-60  
 RL: PRP (Properties)  
 (structural and optical nonlinear properties of Langmuir-Blodgett films  
 of)  
 RN 170646-75-0 CAPLUS  
 CN [5,6]Fullerene-C<sub>60</sub>-1h, 1,9-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX

NAME)

PAGE 1-A



PAGE 2-A



L5 ANSWER 24 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1996:554872 CAPLUS  
 DN 125:275067  
 TI Chemical Generation of C602- and Electron Transfer Mechanism for the  
 Reactions with Alkyl Bromides  
 AU Subramanian, Ramakrishnan; Kadish, Karl M.; Vijayashree, Madakasira N.;  
 Gao, Xiang; Jones, M. Thomas; Miller, Mitchell D.; Krause, Kurt L.;  
 Suenobu, Tomoyoshi; Fukuzumi, Shunichi  
 CS Department of Chemistry, University of Houston, Houston, TX, 77204-5641,  
 USA  
 SO Journal of Physical Chemistry (1996), 100(40), 16327-16335  
 CODEN: JPCHAX; ISSN: 0022-3654  
 PB American Chemical Society  
 DT Journal  
 LA English  
 AB A simple solution-phase method that uses chemical generated p-benzoquinone  
 dianions (Q2-) as the reductant in the selective generation of either  
 C60•- or C602- is described. The electron transfer reduction of C60 by  
 Q2- occurs via stepwise electron transfer from the Q2- to C60 in  
 acetonitrile or benzonitrile. The C602- thus generated is used as the  
 starting material in the synthesis of RxC60 (where x = 2 for R = C6H5CH2  
 and x = 1 for R = o-xyllyl) by the reaction of C602- with benzyl bromide or  
 α,α'-dibromo-o-xylene. Theor. calcns. predict that the  
 1,4-isomer of (C6H5CH2)2C60 should be selectively formed, and this is  
 confirmed by single-crystal x-ray diffraction studies. UV-visible and

near-IR spectroscopy were used to monitor the progress of electron transfer from the Q2- to C60 as well as the subsequent reactions between C602- and the alkyl bromides. The comparison of the observed rate consts. of the reactions of C602- with those of electron transfer from tetramethylsemiquinone radical anion to the same alkyl bromide indicates that the formation of RxC60 proceeds via the rate-determining electron transfer from C602- to the alkyl bromide.

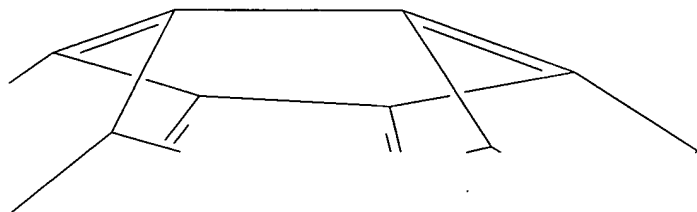
IT 182070-59-3 182070-67-3

RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)  
(chemical generation of C602- and electron transfer mechanism for the reactions with alkyl bromides)

RN 182070-59-3 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,2-dihydro-1-(phenylmethyl)-, ion(1-) (9CI) (CA INDEX NAME)

PAGE 1-A



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

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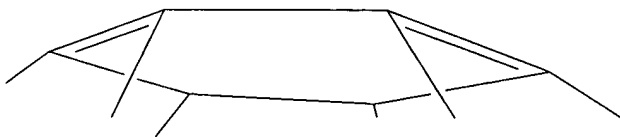
RN 182070-67-3 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1-[[2-(bromomethyl)phenyl]methyl]-1,2-dihydro-,  
ion(1-) (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B





\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

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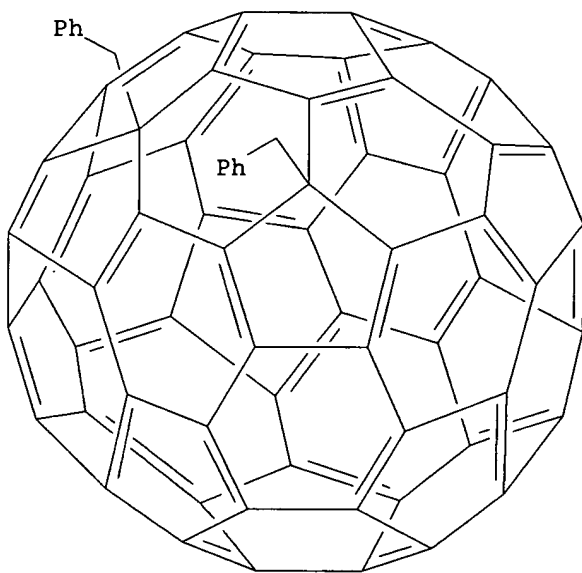
IT 182212-24-4 182212-26-6

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(chemical generation of C602- and electron transfer mechanism for the reactions with alkyl bromides)

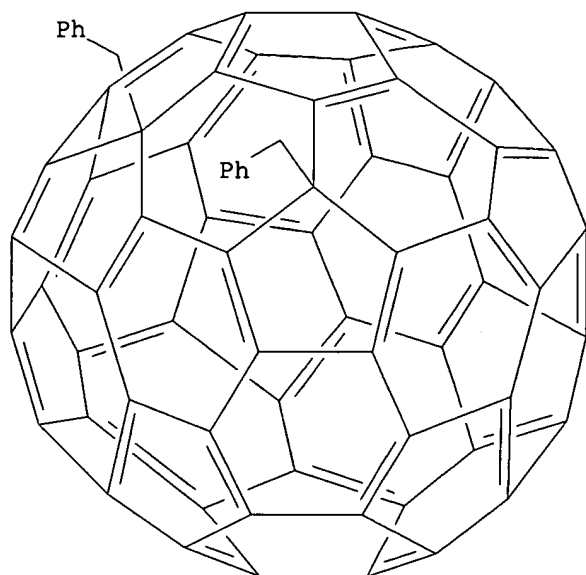
RN 182212-24-4 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-dihydro-1,7-bis(phenylmethyl)-, radical ion(1-)  
(9CI) (CA INDEX NAME)



RN 182212-26-6 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,7-dihydro-1,7-bis(phenylmethyl)-, radical ion(2-)  
(9CI) (CA INDEX NAME)



IT 172885-95-9 172990-44-2

RL: PRP (Properties)

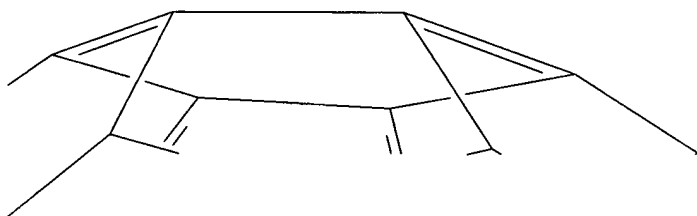
(chemical generation of C60<sup>2-</sup> and electron transfer mechanism for the reactions with alkyl bromides)

RN 172885-95-9 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,2-dihydro-1,2-bis(phenylmethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

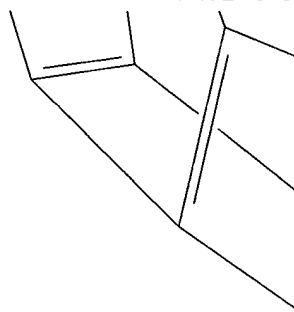
PAGE 1-B



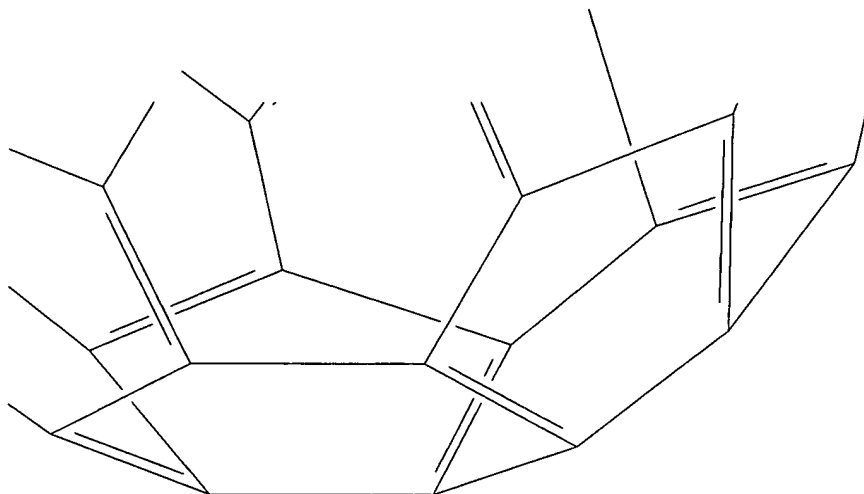
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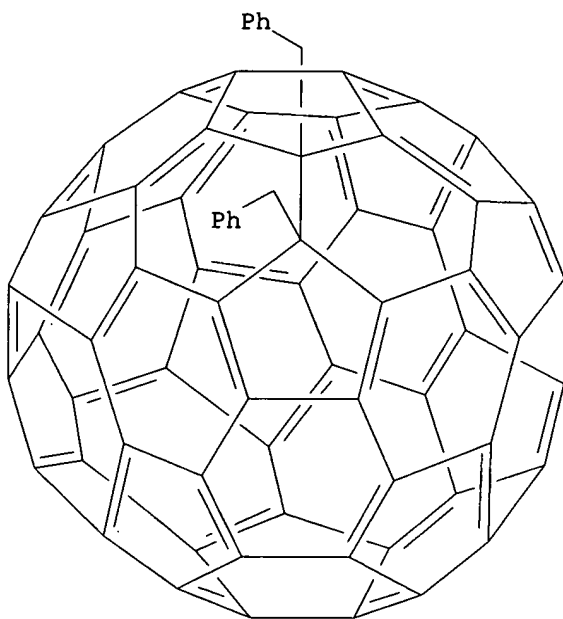
PAGE 3-A



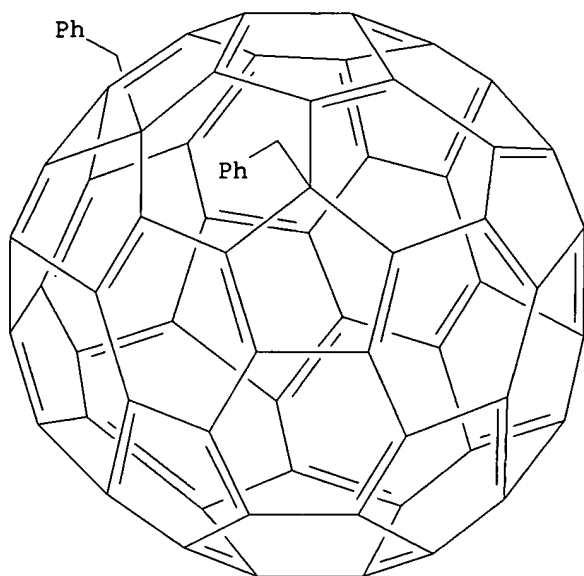
PAGE 3-B



RN 172990-44-2 CAPLUS  
 CN [5,6]Fullerene-C60-Ih, 1,9-dihydro-1,9-bis(phenylmethyl)- (9CI) (CA INDEX NAME)

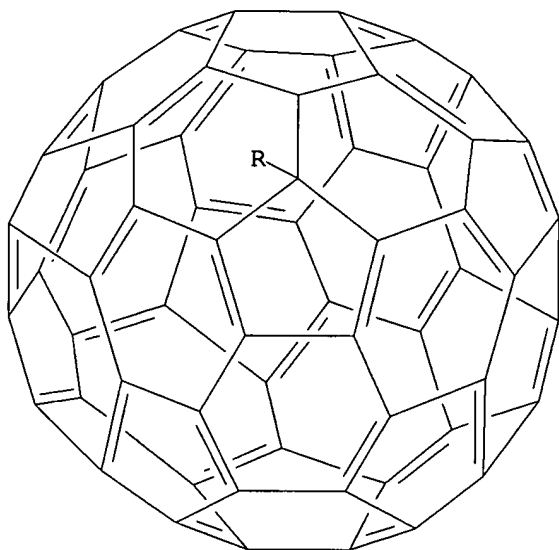


IT **176106-61-9P**  
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)  
 (crystal and mol. structure; chemical generation of C602- and electron transfer mechanism for the reactions with alkyl bromides)  
 RN 176106-61-9 CAPLUS  
 CN [5,6]Fullerene-C60-Ih, 1,7-dihydro-1,7-bis(phenylmethyl)- (9CI) (CA INDEX NAME)

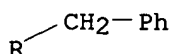


L5 ANSWER 25 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1996:356136 CAPLUS  
 DN 125:114273  
 TI Unusual reactions of C<sub>60</sub> with aldehydes in the presence of aqueous ammonia  
 AU Komori, Akifumi; Kubota, Masayuki; Ishida, Takayuki; Niwa, Haruki; Nogami, Takashi  
 CS Dep. Appl. Phys. Chem., Univ. Electro-Commun., Chofu, 182, Japan  
 SO Tetrahedron Letters (1996), 37(23), 4031-4034  
 CODEN: TELEAY; ISSN: 0040-4039  
 PB Elsevier  
 DT Journal  
 LA English  
 OS CASREACT 125:114273  
 AB Fullerene C<sub>60</sub> reacts with alkylaldehydes in the presence of aqueous ammonia to give 2,5-dialkyl-substituted pyrrolidine derivs. The reaction of phenylacetaldehyde under similar conditions afforded C<sub>60</sub>(H)(CH<sub>2</sub>Ph) via possible decarbonylation. On the basis of the product anal., reaction mechanisms are proposed in which C<sub>60</sub> plays the role of a dipolarophile or radical scavenger.  
 IT **170646-75-0P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (unusual reactions of C<sub>60</sub> with aldehydes in the presence of aqueous ammonia)  
 RN 170646-75-0 CAPLUS  
 CN [5,6]Fullerene-C<sub>60</sub>-1h, 1,9-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



L5 ANSWER 26 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1996:212770 CAPLUS  
 DN 124:342817  
 TI Fullerene-acetylene hybrids: towards a novel class of molecular carbon  
 allotropes  
 AU Timmerman, Peter; Anderson, Harry L.; Faust, Ruediger; Nierengarten,  
 Jean-Francois; Habicher, Tilo; Seiler, Paul; Diederich, Francois  
 CS Lab. Org. Chem., ETH-Zentrum, Zurich, CH-8092, Switz.  
 SO Tetrahedron (1996), 52(14), 4925-47  
 CODEN: TETRAB; ISSN: 0040-4020  
 PB Elsevier  
 DT Journal  
 LA English  
 OS CASREACT 124:342817  
 AB The synthesis and complete characterization of 17 new fullerene-acetylene  
 covalent derivs. is described. Reaction of 3-bromo-1,5-  
 bis(trimethylsilyl)penta-1,4-diyne with C60 gave bis-protected  
 diethynylmethanofullerene (4) in 56% yield. Unsym. bis-protected  
 diethynylmethanofullerene (6) was synthesized in 53% yield from  
 tosylhydrazone [(i-Pr)3SiC.tplbond.CC(:NNHTos)C.tplbond.CSiMe3] and C60.  
 Proto-desilylation of 4 and 6 gave the corresponding free alkynes (3 and  
 8) in 83% and 69% yield, resp. Partial deprotection of 4 afforded the  
 mono-protected fullerene in 35% yield. Oxidative hetero-coupling  
 reactions of 3 and 8 under Hay conditions with various monosubstituted  
 acetylenes gave butadiynylmethanofullerenes (10-13) in yields varying from  
 25-49%. Homo-coupling of 8 produced dumbbell-shaped fullerene 14, the 1st  
 dimeric fullerene that could be fully characterized. The x-ray crystal

structure anal. of 14 revealed little or no electronic interaction between the two fullerene spheres. Addition of lithium trimethylsilylacetylide to C60 gave access to 1-substituted-2-(trimethylsilylethynyl)fullerenes. The acidity of hydro(trimethylsilylethynyl)fullerene (16), synthesized in 58% yield, was studied as a function of base and solvent. Reaction of lithiated (trimethylsilylethynyl)fullerene (17) with various electrophiles is discussed. Alc. (trimethylsilylethynyl)fullerenemethanol (25) was prepared in 57% yield by reaction of 17 with formaldehyde. Under strongly basic conditions, 25 eliminates formaldehyde to give 16 in quant. yield. Oxidation of 25 afforded (trimethylsilylethynyl)fullerenecarboxaldehyde in 53% yield, a rather unstable compound that is easily converted to hydrofullerene 16. Conversion of 25 to the corresponding tosylate could be performed in 40% yield.

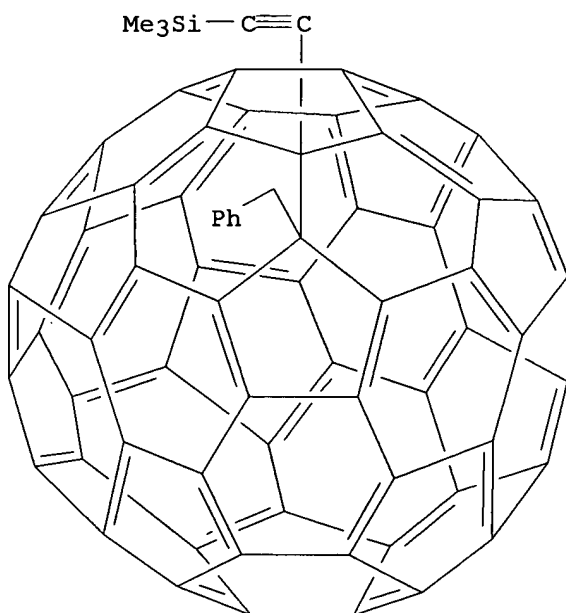
IT **175874-71-2P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of fullerene-acetylene derivs.)

RN 175874-71-2 CAPLUS

CN Silane, trimethyl[[9-(phenylmethyl)[5,6]fulleren-C60-1h-1(9H)-yl]ethynyl]- (9CI) (CA INDEX NAME)

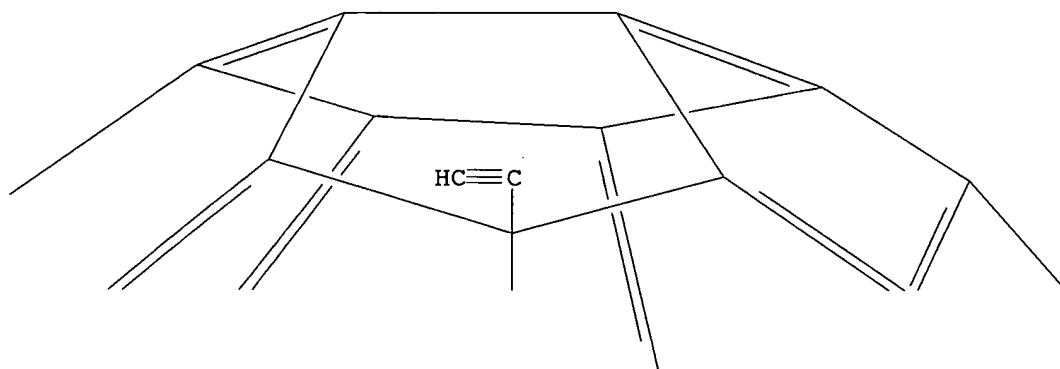


IT **175874-75-6P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of fullerene-acetylene derivs.)

RN 175874-75-6 CAPLUS

CN [5,6]Fullerene-C60-1h, 1-ethynyl-1,9-dihydro-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



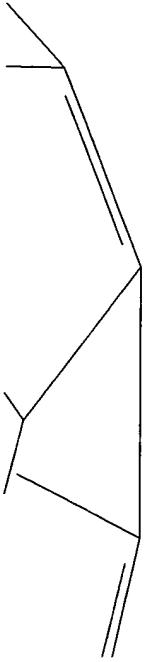


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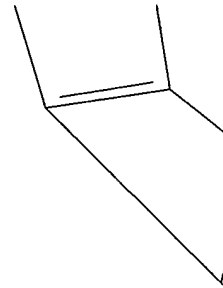
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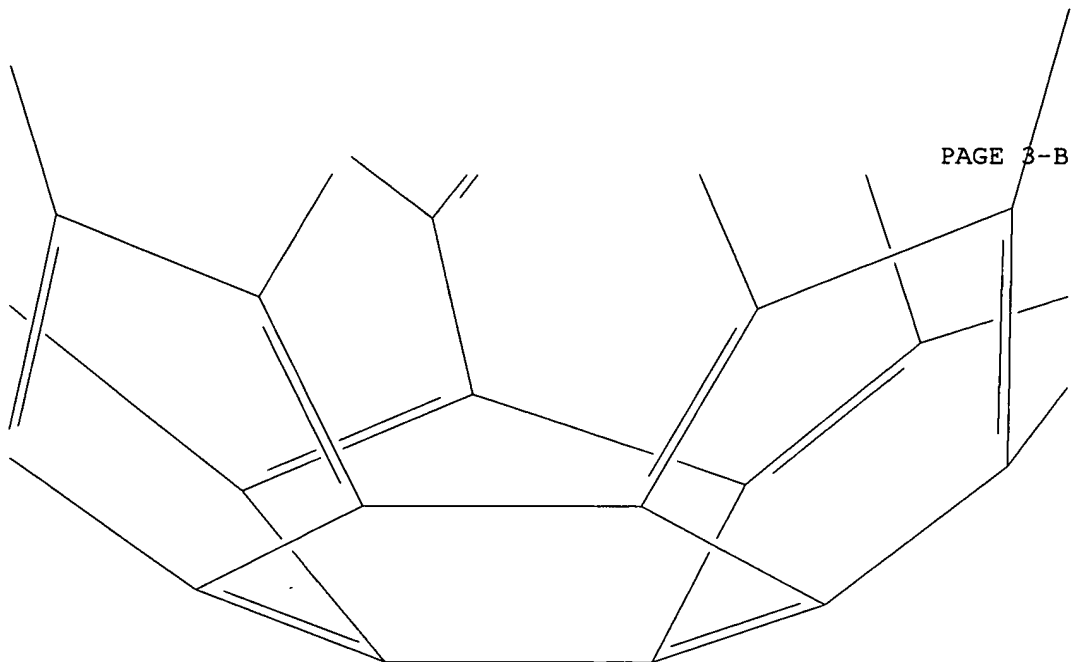
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

PAGE 2-C



PAGE 3-A





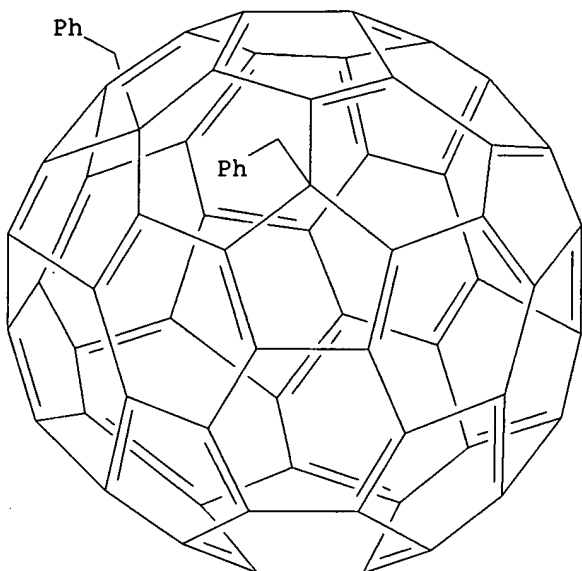
PAGE 3-C

L5 ANSWER 27 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1996:182541 CAPLUS  
DN 124:316718  
TI Introduction of two benzyl groups to C60 by using the Collman reagent  
AU Miki, Sadao; Kitao, Masunori; Fukunishi, Koushi  
CS Dep. Chemistry, Kyoto Inst. Technol., Kyoto, 606, Japan  
SO Tetrahedron Letters (1996), 37(12), 2049-52  
CODEN: TELEAY; ISSN: 0040-4039  
PB Elsevier  
DT Journal  
LA English  
OS CASREACT 124:316718  
AB Addition of C60 to a suspension of the Collman reagent in THF gave a strongly colored but almost transparent solution. Treatment of the resulting solution with benzyl bromide gave a C60 derivative possessing two benzyl groups. The 1H-NMR as well as the 13C-NMR of the product indicated that the reaction site was 1,4-position.  
IT 176106-61-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(fullerene benzylation using Collman's reagent)

RN 176106-61-9 CAPLUS

CN [5,6]Fullerene-C60-1h, 1,7-dihydro-1,7-bis(phenylmethyl)- (9CI) (CA INDEX NAME)



L5 ANSWER 28 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1996:127530 CAPLUS

DN 124:288947

TI Fullerene-acetylene molecular scaffolding: chemistry of 2-functionalized 1-ethynylated C60, oxidative homocoupling, hexakis-adduct formation, and attempted synthesis of C1242-

AU Timmerman, Peter; Witschel, Lars E.; Diederich, Francois; Boudon, Corinne; Gisselbrecht, Jean-Paul; Gross, Maurice

CS Lab. Org. Chem., ETH-Zentrum, Zurich, CH-8092, Switz.

SO Helvetica Chimica Acta (1996), 79(1), 6-20

CODEN: HCACAV; ISSN: 0018-019X

PB Verlag Helvetica Chimica Acta

DT Journal

LA English

AB On the way to the fullerene-acetylene hybrid carbon allotropes, the oxidative homocoupling of 2-functionalized 1-ethynylated C60 derivs. was investigated. Under Glaser-Hay conditions, two soluble dumbbell-shaped bisfullerenes with two C60 moieties 2,2'-substituted by PhCH2 or CH2OR (R = tetrahydropyranyl; I) linked by a butadiynediyl bridge were formed in 52 and 82% yield, resp. Cyclic-voltammetric measurements revealed that there is no significant electronic communication between the two fullerene spheres via the butadiynediyl linker. Removal of the protective groups in I gave in 80% yield a highly insol. dumbbell with methanol groups in the 2,2'-positions of the butadiynediyl-bridged carbon spheres. Attempted conversion of this compound to the corresponding all-carbon dianion C1242- via base-induced elimination of formaldehyde was not successful presumably due to exo-dig cyclization of the formed alkoxides. The occurrence of this cyclization under furan formation was proven for the soluble model

compound 2-[4-(trimethylsilyl)buta-1,3-dien-1-yl][60]fullerene-1-methanol. To compare the properties of ethynylated fullerene mono-adducts to those of corresponding higher adducts, two hexakis-adducts with an octahedral functionalization pattern resulting from all-equatorial addns. were prepared by the reversible-template method of Hirsch. Reaction of ethynylated mono-adducts with 2-bromomalonate/DBU in the presence of 1,9-dimethylantracene as reversible template led to hexakis-adducts in 28 and 22% yield. Preliminary expts. indicated a significant change in reactivity and NMR spectral properties of the fullerene addends with increasing degree of functionalization.

IT **175874-75-6**

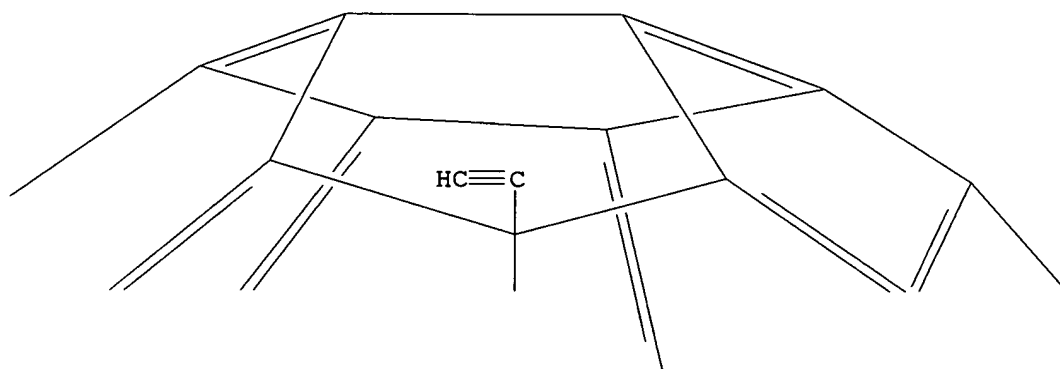
RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of butadiynediyl-linked bisfullerenes and attempted conversion to dianion)

RN 175874-75-6 CAPLUS

CN [5,6]Fullerene-C60-1h, 1-ethynyl-1,9-dihydro-9-(phenylmethyl)- (9CI) (CA INDEX NAME)

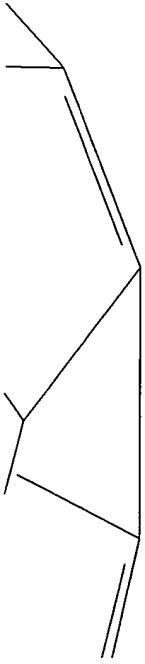
PAGE 1-A



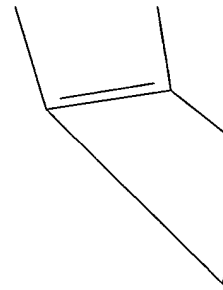
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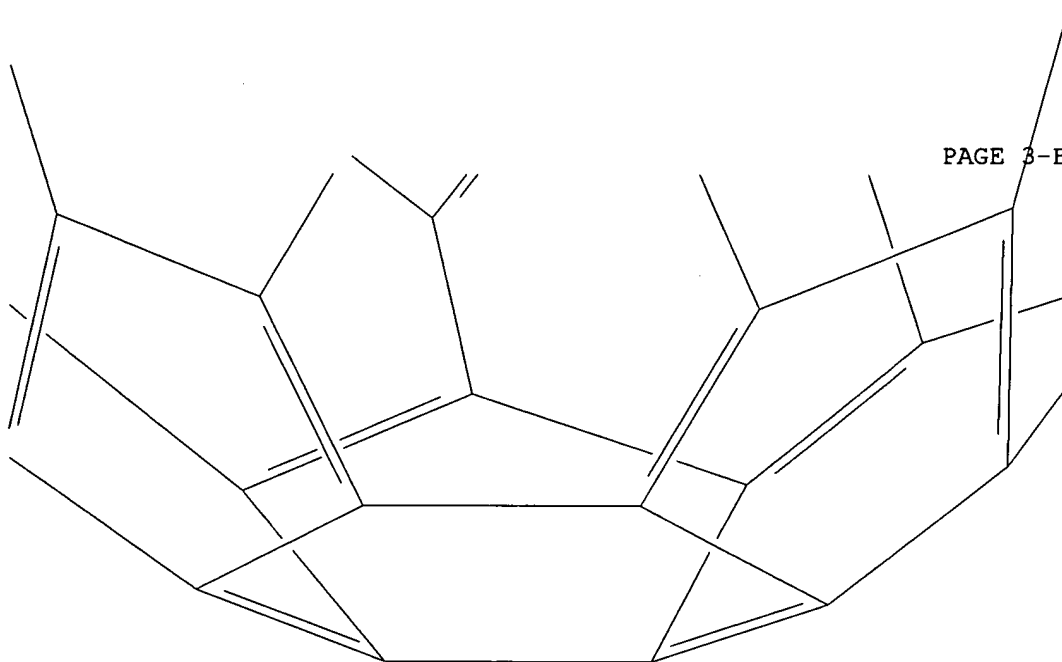
PAGE 2-C



PAGE 3-A

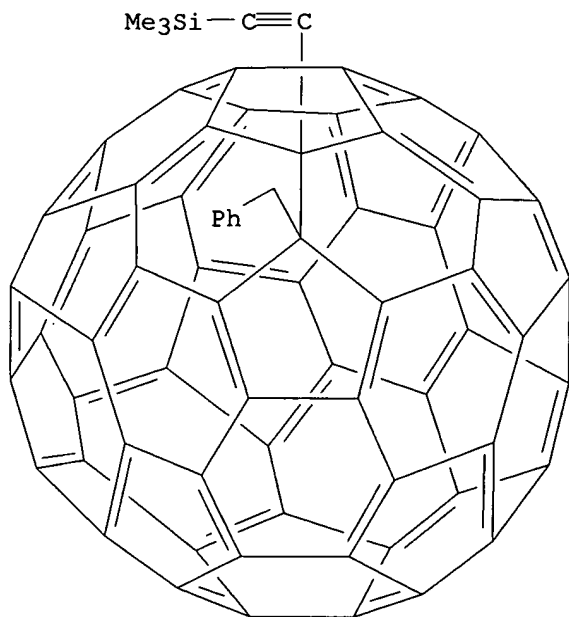






PAGE 3-C

IT **175874-71-2P 175874-76-7P**  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (reduction potential; preparation of butadiynediyl-linked bisfullerenes and  
 attempted conversion to dianion)  
 RN 175874-71-2 CAPLUS  
 CN Silane, trimethyl[[9-(phenylmethyl)[5,6]fulleren-C60-1h-1(9H)-yl]ethynyl]-  
 (9CI) (CA INDEX NAME)



RN 175874-76-7 CAPLUS  
 CN [5,6]Fullerene-C60-Ih, 1,1'-(1,3-butadiyne-1,4-diyl)bis[1,9-dihydro-9-(phenylmethyl)-(9CI) (CA INDEX NAME)

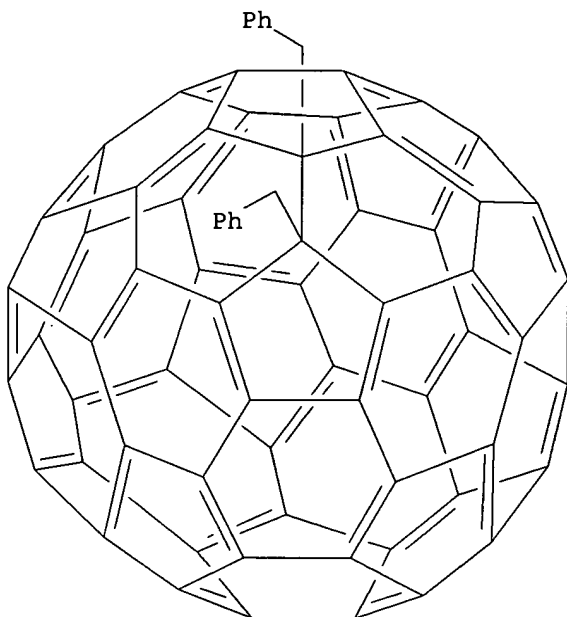
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L5 ANSWER 29 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1995:991561 CAPLUS  
 DN 124:116838  
 TI Synthesis and characterization of (C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>2</sub>C<sub>60</sub> and related derivatives  
 AU Subramanian, R.; Vijayashree, M. N.; Mead, S. L.; Gao, X.; Jones, M. T.;  
 Kadish, K. M.; Suenobu, T.; Fukuzumi, S.  
 CS Dep. Chem., Univ. Houston, Houston, TX, 77204-5641, USA  
 SO Proceedings - Electrochemical Society (1995), 95-10 (Proceedings  
 of the Symposium on Recent Advances in the Chemistry and Physics of  
 Fullerenes and Related Materials, 1995), 1150-63  
 CODEN: PESODO; ISSN: 0161-6374  
 PB Electrochemical Society  
 DT Journal  
 LA English  
 AB A simple, solution-phase chemical method which uses chemical generated  
 hydroquinone dianion as a reductant in the selective generation of either C<sub>60</sub>- or C<sub>60</sub><sup>2-</sup>  
 is described. The C<sub>60</sub><sup>2-</sup> thus generated was used as the starting material  
 in the synthesis of RxC<sub>60</sub> where x = 2 for R = C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub> and x = 1 for R =  
 o-xylyl. The products were characterized by <sup>1</sup>H NMR spectroscopy which  
 suggests that in the case of (C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>2</sub>C<sub>60</sub>, only the 1,2-isomer (and not  
 the thermodynamically favored 1,4-isomer) was obtained. UV-visible and  
 near-IR spectroscopy were used to monitor the progress of electron  
 transfer from the hydroquinone dianion to C<sub>60</sub> as well as the subsequent  
 reaction between C<sub>60</sub><sup>2-</sup> and the alkyl halide. Based on these results, a  
 three step mechanism for the formation of RxC<sub>60</sub> is proposed.  
 IT 172990-44-2P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(preparation and electrochem. reduction potentials of)

RN 172990-44-2 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,9-dihydro-1,9-bis(phenylmethyl)- (9CI) (CA INDEX NAME)



L5 ANSWER 30 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1995:991467 CAPLUS

DN 124:129665

TI Electrochemistry, near-IR and ESR spectroscopy of (R)<sub>x</sub>C<sub>60</sub> where R = H, CH<sub>3</sub>, C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub> or o-xyllyl

AU Kadish, Karl M.; Boulas, Pierre L.; Vijayashree, M. N.; Subramanian, Ramakrishnan; Gao, Xiang; Mead, Steve; Tan, Zheng; Jones, M. Thomas  
 CS Department Chemistry, University Houston, Houston, TX, 77204-5641, USA  
 SO Proceedings - Electrochemical Society (1995), 95-10 (Proceedings of the Symposium on Recent Advances in the Chemistry and Physics of Fullerenes and Related Materials, 1995), 213-28

CODEN: PESODO; ISSN: 0161-6374

PB Electrochemical Society

DT Journal

LA English

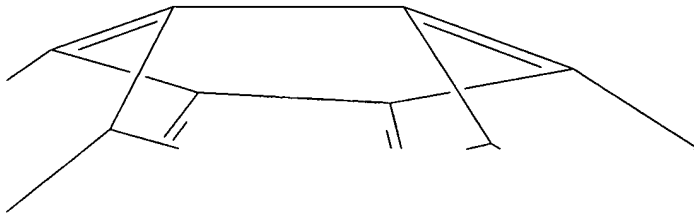
AB The authors report here the electrochem., near-IR and ESR spectroscopy of fullerene derivs. (R)<sub>x</sub>C<sub>60</sub> where x = 2 or 4 in the case of R = H, CH<sub>3</sub> and C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>, and x = 1 or 2 in the case of R = o-xyllyl. The electrochem. properties of organofullerenes depend upon factors such as temperature and solvent as well as upon the number and type of addends. The near-IR absorption and ESR spectra of selected electroreduced (R)<sub>x</sub>C<sub>60</sub> derivs. show similar ESR spectra which originate from at least two different types of radicals. The temperature dependence of the [(R)<sub>x</sub>C<sub>60</sub>]-spectra might be consistent with the formation of dimers.

IT 172885-99-3 173006-79-6

RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)

(electrochem. formation and electrochem. reduction in various solvents)  
RN 172885-99-3 CAPLUS  
CN [5,6]Fullerene-C60-Ih, 1,2-dihydro-1,2-bis(phenylmethyl)-, radical ion(1-)  
(9CI) (CA INDEX NAME)

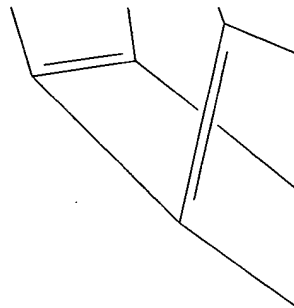
PAGE 1-A

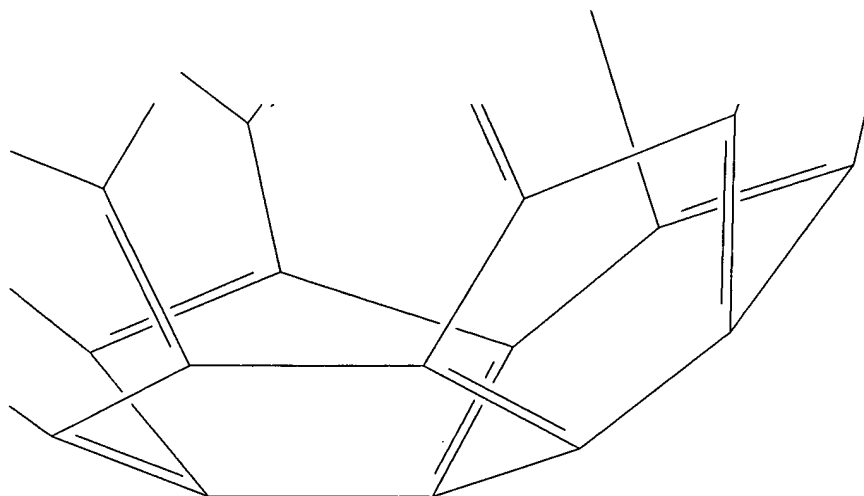


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PAGE 3-A

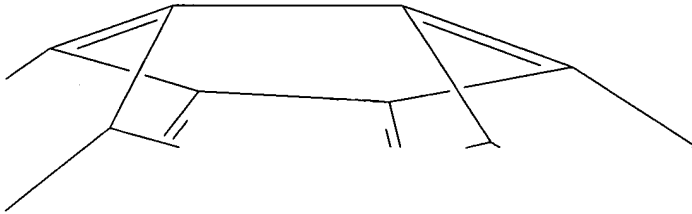




PAGE 3-B

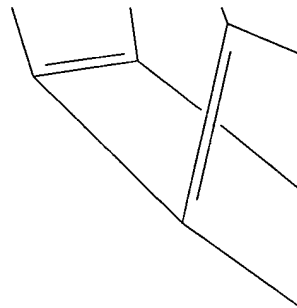
RN 173006-79-6 CAPLUS  
CN [5,6]Fullerene-C60-Ih, 1,2-dihydro-1,2-bis(phenylmethyl)-, radical ion(2-)  
(9CI) (CA INDEX NAME)

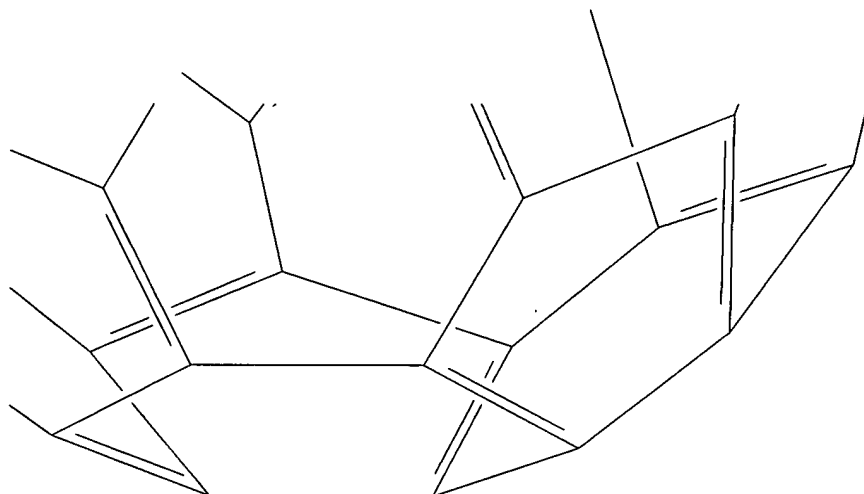
PAGE 1-A



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PAGE 3-B

IT **172885-95-9**

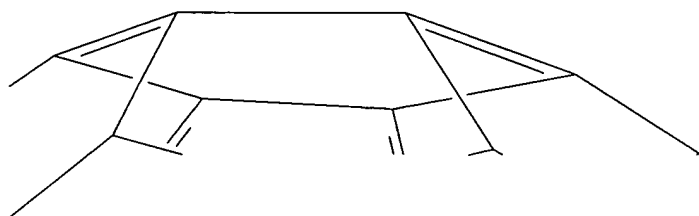
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)  
(electrochem. reduction in various solvents)

RN 172885-95-9 CAPLUS

CN [5,6]Fullerene-C60-Ih, 1,2-dihydro-1,2-bis(phenylmethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

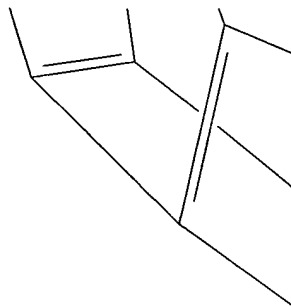


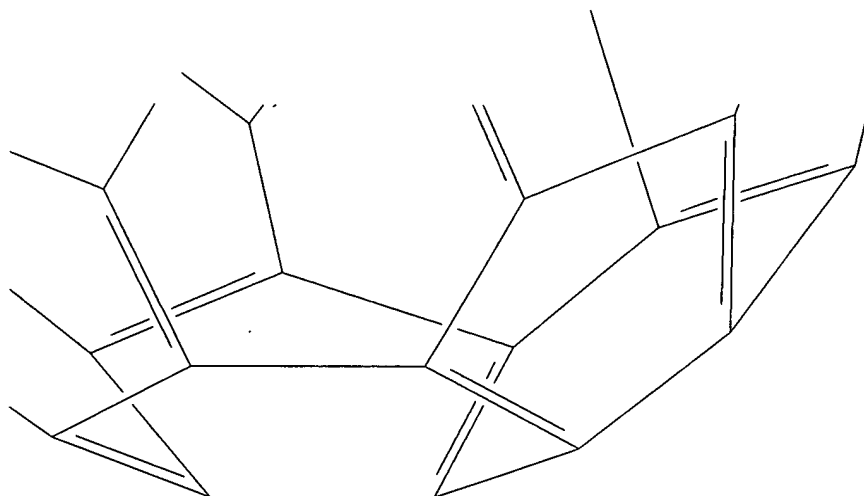


\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

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PAGE 3-A

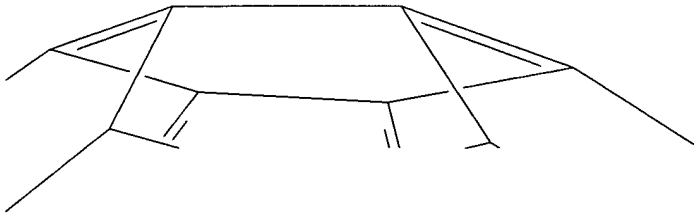




PAGE 3-B

IT **173006-81-0**  
 RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)  
 (electrochem. reductive formation and half-wave potential of)  
 RN 173006-81-0 CAPLUS  
 CN [5,6]Fullerene-C60-Ih, 1,2-dihydro-1,2-bis(phenylmethyl)-, radical ion(3-)  
 (9CI) (CA INDEX NAME)

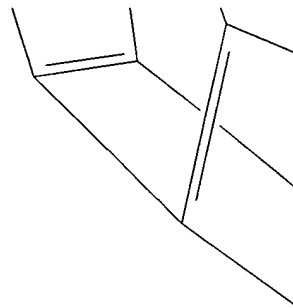
PAGE 1-A

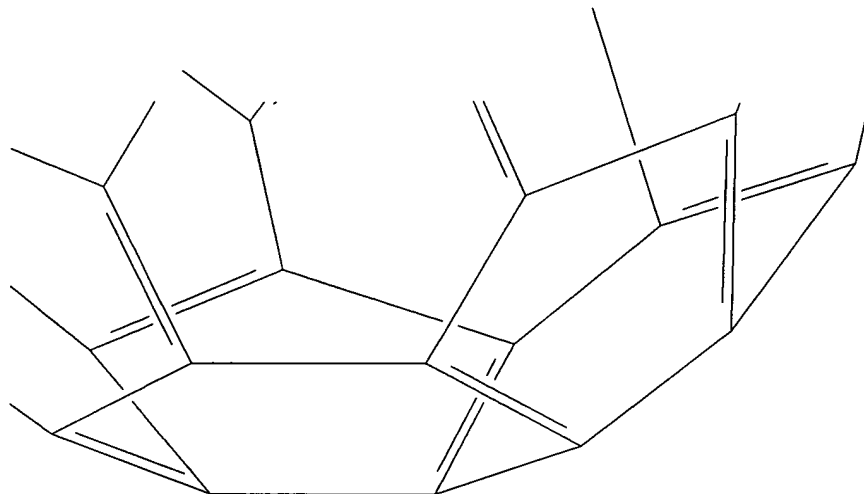


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PAGE 3-A





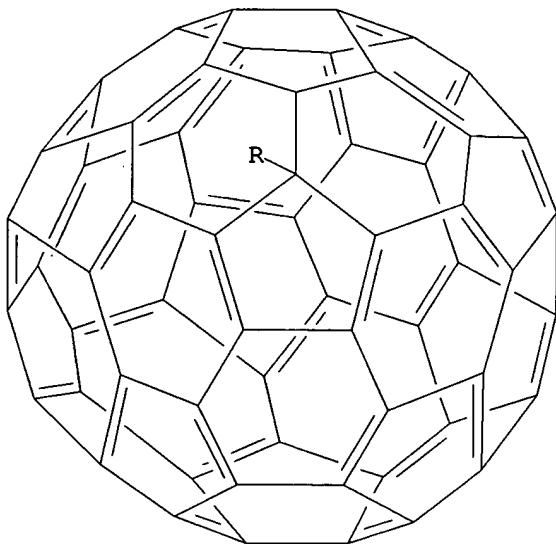
L5 ANSWER 31 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1995:899337 CAPLUS  
 DN 123:313538  
 TI Cyanodihydrofullerenes and Dicyanodihydrofullerene: The First Polar Solid Based on C60  
 AU Keshavarz-K, Majid; Knight, Brian; Srdanov, Gordana; Wudl, Fred  
 CS Institute for Polymers and Organic Solids, University of California, Santa Barbara, CA, 93106-5090, USA  
 SO Journal of the American Chemical Society (1995), 117(45), 11371-2  
 CODEN: JACSAT; ISSN: 0002-7863  
 PB American Chemical Society  
 DT Journal  
 LA English  
 OS CASREACT 123:313538  
 AB The authors describe the synthesis of 1-cyano-2-protio dihydrofullerene (2), 1-cyano-2-Me dihydrofullerene (3), 1-cyano-2-p-tert-butylbenzyl dihydrofullerene (4), and 1,2-dicyano dihydrofullerene (5). The 1st crystal structural of any dihydrofullerene, in this case 5, is described. Surprisingly, it forms a polar solid with the nitrile dipoles pointing along the crystallog. b axis and also, the sp<sup>3</sup> hybridized carbon atoms have very nearly tetrahedral angles (108.8°). 5 Has a 1st reduction wave 120 mV more pos. than C60.  
 IT **170244-42-5P**  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and electrochem. reduction)  
 RN 170244-42-5 CAPLUS  
 CN [5,6]Fullerene-C60-Ih-1(9H)-carbonitrile, 9-[[4-(1,1-dimethylethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

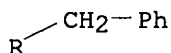
L5 ANSWER 32 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1995:733939 CAPLUS  
 DN 123:339357  
 TI Isomerically pure organo[60]fullerenes from C602- salt: synthesis and characterization of 1-benzyl-2-hydro[60]fullerene

AU Chen, Jian; Cai, Rui-Fang; Huang, Zu-En; Wu, Hou-Ming; Jiang, Shao-Kai;  
Shao, Qian-Fen  
CS Dep. Chem., Fudan Univ., Shanghai, 200433, Peop. Rep. China  
SO Journal of the Chemical Society, Chemical Communications (1995),  
(15), 1553-4  
CODEN: JCCCAT; ISSN: 0022-4936  
PB Royal Society of Chemistry  
DT Journal  
LA English  
OS CASREACT 123:339357  
AB Isomerically pure 1-benzyl-2-hydro[60]fullerene is synthesized in 64%  
yield by the reaction of C60<sup>2-</sup> potassium salt with benzyl chloride in THF  
at 50°C.  
IT **170646-75-0P**  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(synthesis and characterization of 1-benzyl-2-hydro[60]fullerene)  
RN 170646-75-0 CAPLUS  
CN [5,6]Fullerene-C60-Ih, 1,9-dihydro-1-(phenylmethyl)- (9CI) (CA INDEX  
NAME)

PAGE 1-A



PAGE 2-A



L5 ANSWER 33 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1995:713519 CAPLUS  
DN 123:313537  
TI Photolysis of o-methylbenzophenone in the presence of C60. Facile cleavage  
of the C-C bond connected to C60  
AU Tomioka, Hideo; Ichihashi, Masaki; Yamamoto, Katsutoshi  
CS Chemistry Dep. Materials, Mie Univ., Mie, 514, Japan

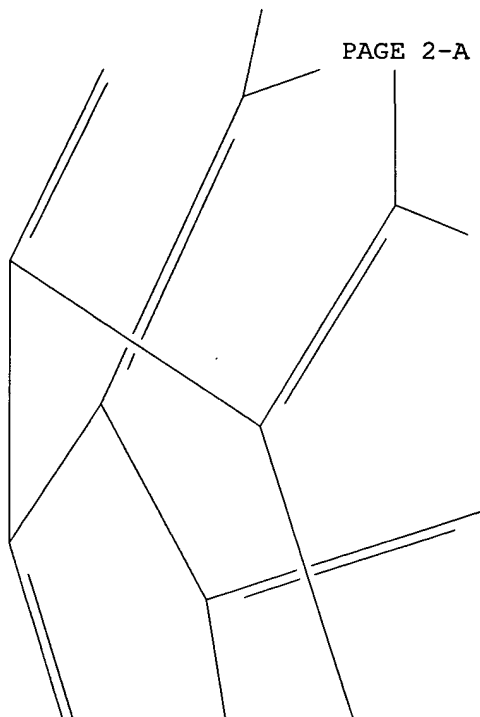
SO Tetrahedron Letters (1995), 36(30), 5371-4  
 CODEN: TELEAY; ISSN: 0040-4039  
 PB Elsevier  
 DT Journal  
 LA English  
 OS CASREACT 123:313537  
 GI For diagram(s), see printed CA Issue.  
 AB Irradiation of the title ketone with C60 gave 61-hydroxy-61-phenyl-1,9-(methano[1,2]benzenomethano)fullerene (I) (A = 6,6 bond substituted fullerene C60 moiety) as a result of Diels-Alder addition of 7-hydroxy-7-phenyl-o-quinodimethane with C60: the adduct is shown to undergo facile cleavage of the C-C bond connected to C60 either by silica gel chromatog. or upon heating in toluene to produce 1-(2-benzoylphenyl)methyl-1,2-dihydrofullerene (II).  
 IT **169964-19-6P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (photolysis of o-methylbenzophenone in the presence of C60, and facile cleavage of the C-C bond connected to C60)  
 RN 169964-19-6 CAPLUS  
 CN Methanone, [2-([5,6]fulleren-C60-Ih-1(9H)-ylmethyl)phenyl]phenyl- (9CI)  
 (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

L5 ANSWER 34 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1995:192398 CAPLUS  
 DN 122:91357  
 TI Reversible reduction potentials of some new organofullerenes  
 AU Evans, Dennis H.; Lerke, Susan A.  
 CS Department Chemistry and Biochemistry, University Delaware, Newark, DE, 19716, USA  
 SO Proceedings - Electrochemical Society (1994), 94-24 (Recent Advances in the Chemistry and Physics of Fullerenes and Related Materials), 1087-97  
 CODEN: PESODO; ISSN: 0161-6374  
 DT Journal  
 LA English  
 AB Reversible potentials for the 1st 3 steps of reduction of 1,2-xylenediyl-, 1-methyl-4-t-butyl- and 1-benzyl-4-t-butyl-C60 in THF are reported. Each potential for these compds. is shifted .apprx.0.1 V in the neg. direction compared to the corresponding potentials of the parent fullerene. Published data for related compds. are reviewed, and the results are discussed in relation to those obtained with aromatic hydrocarbon analogs.  
 IT **160482-48-4**, 1-Benzyl-4-t-butylfullerene(C60)  
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)  
 (reversible reduction potentials of new organofullerenes)  
 RN 160482-48-4 CAPLUS  
 CN [5,6]Fullerene-C60-Ih, 1-(1,1-dimethylethyl)-1,7-dihydro-7-(phenylmethyl)- (9CI) (CA INDEX NAME)

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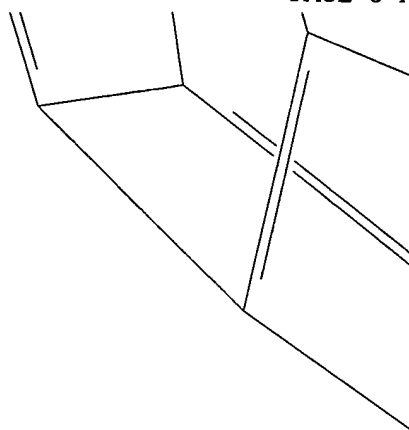
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*



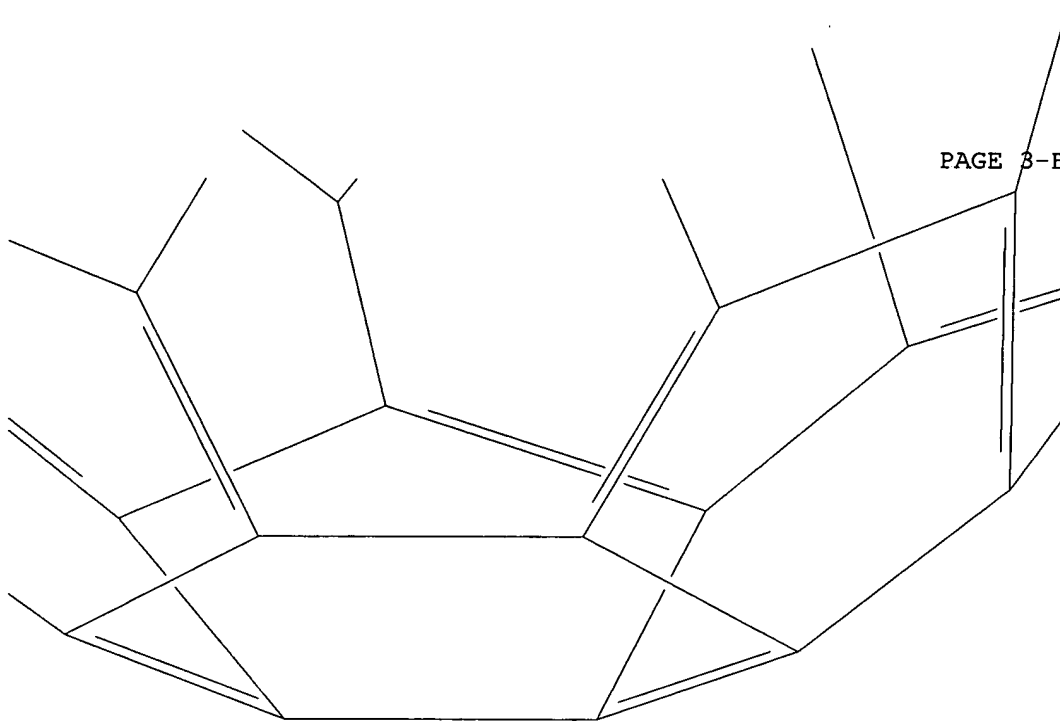
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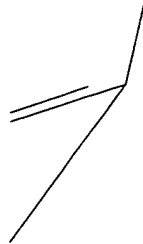
PAGE 3-A



PAGE 3-B







L5 ANSWER 35 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1994:482375 CAPLUS  
 DN 121:82375  
 TI Addition of alkyl radicals to C60. Part 3. The EPR spectra of R3C60 radicals and a theoretical study of HC60 and H3C60 radicals  
 AU Morton, J. R.; Negri, F.; Preston, K. F.  
 CS Steacie Inst. Mol. Sci., Natl. Res. Counc. Canada, Ottawa, ON, K1A 0R6, Can.  
 SO Canadian Journal of Chemistry (1994), 72(3), 776-82  
 CODEN: CJCHAG; ISSN: 0008-4042  
 DT Journal  
 LA English  
 AB The EPR spectra of a series of C60 adducts of the type R3C60 are described and discussed. In every case, two of the three ligands are equivalent, leading to the conclusion that the R3C60 radicals have a plane of symmetry. The unpaired electron distributions in mono- and trisubstituted-C60 radicals are computed with the help of the QCFF/PI and MNDO Hamiltonians. It is shown that the hyperfine consts. predicted on the basis of the calculated spin densities reproduce well the values observed and suggest a reassignment of framework 13C coupling consts. in RC60.  
 IT **140700-29-4P**  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and ESR spectrum of)  
 RN 140700-29-4 CAPLUS  
 CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 10,14-dihydro-2,10,14-tris(phenylmethyl)-(9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

L5 ANSWER 36 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1994:234435 CAPLUS  
 DN 120:234435  
 TI ESR hyperfine patterns for the radicals derived from C60 and C70  
 AU Balasubramanian, K.  
 CS Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ, 85287-1604, USA  
 SO Chemical Physics Letters (1993), 210(1-3), 153-8  
 CODEN: CHPLBC; ISSN: 0009-2614  
 DT Journal  
 LA English  
 AB Theor. ESR hyperfine patterns for the radicals derived from C60 and C70 fullerenes are obtained from combinatorial techniques based on the group-theor. generating functions. Computerized combinatorial methods are

used to obtain simulated ESR hyperfine patterns. The ESR hyperfine patterns for several RnC60 radicals are obtained and compared with experiment

IT **150733-25-8 154362-77-3**

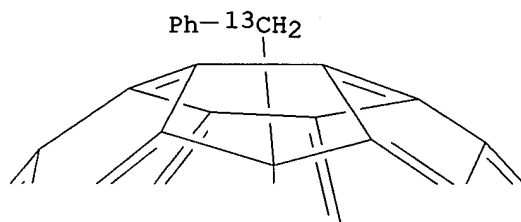
RL: PRP (Properties)

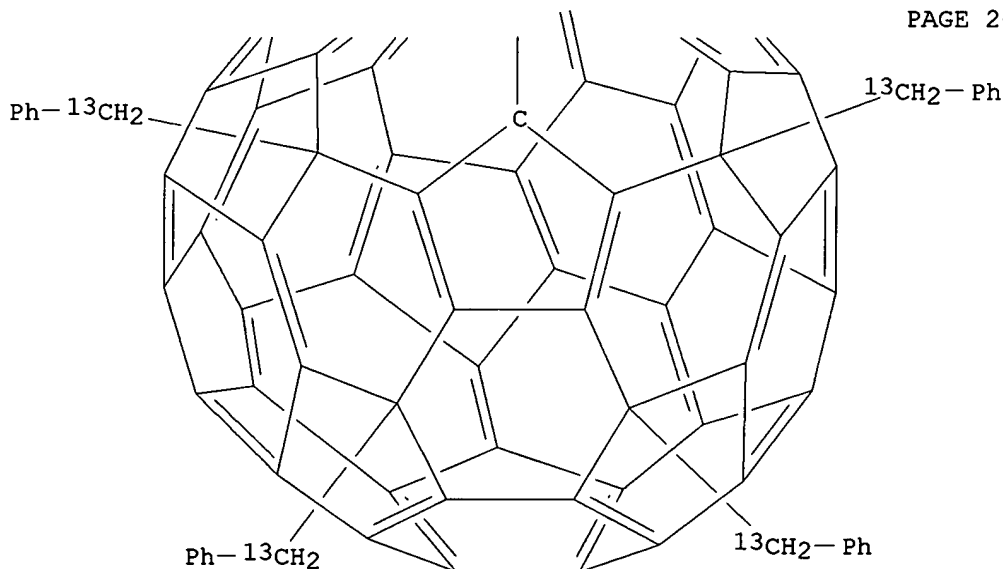
(ESR hyperfine pattern of)

RN 150733-25-8 CAPLUS

CN [5,6]Fulleren-C60-Ih-1(9H)-yl, 6,9,12,15,18-pentakis(phenylmethyl- $^{13}\text{C}$ )-(9CI) (CA INDEX NAME)

PAGE 1-A



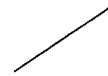


RN 154362-77-3 CAPLUS  
 CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 10,14-dihydro-2,10,14-tris(phenylmethyl-13C)-(9CI) (CA INDEX NAME)

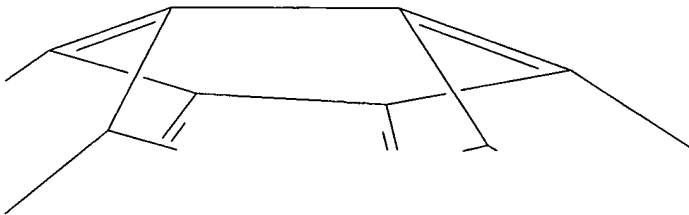
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L5 ANSWER 37 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1993:147000 CAPLUS  
 DN 118:147000  
 TI Radical adducts of fullerenes C60 and C70 studied by laser flash photolysis and pulse radiolysis  
 AU Dimitrijevic, Nada M.; Kamat, Prashant V.; Fessenden, Richard W.  
 CS Radiat. Lab., Univ. Notre Dame, Noret Dame, IN, 46556, USA  
 SO Journal of Physical Chemistry (1993), 97(3), 615-18  
 CODEN: JPCHAX; ISSN: 0022-3654  
 DT Journal  
 LA English  
 AB The reaction of R• (I; R = PhCH<sub>2</sub>, Me<sub>3</sub>C, Cl<sub>3</sub>C, Cl<sub>2</sub>CH) with C<sub>60</sub> and C<sub>70</sub> was examined using laser flash photolysis and pulse radiolysis. The alkyl radicals are very reactive toward fullerenes and form radical adducts, (RC<sub>60</sub>)• and (RC<sub>70</sub>)•. The difference absorption spectrum of (RC<sub>60</sub>)• exhibits broad absorption in the visible; that of (RC<sub>70</sub>)• exhibits bleaching of absorption in the region 440-560 nm. The rate consts. for the reaction of these radicals with fullerenes are in the range of 10<sup>8</sup> M<sup>-1</sup> s<sup>-1</sup> for I (R = Cl<sub>2</sub>CH) to diffusion controlled for I (R = Me<sub>3</sub>C).  
 IT **140656-83-3**  
 RL: PRP (Properties)  
 (UV of)  
 RN 140656-83-3 CAPLUS  
 CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 2-(phenylmethyl)-(9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



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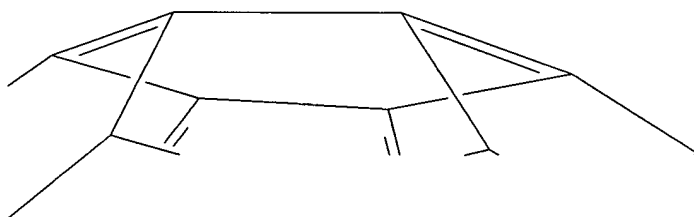
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

L5 ANSWER 38 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1993:59182 CAPLUS  
 DN 118:59182  
 TI Electron paramagnetic resonance spectra of fullerene R-C60 radicals.  
 Evidence for RC60C60R dimers  
 AU Morton, J. R.; Preston, K. F.; Krusic, P. J.; Wasserman, E.  
 CS Steacie Inst. Mol. Sci., Natl. Res. Counc. Canada, Ottawa, ON, K1A 0R9,  
 Can.  
 SO Journal of the Chemical Society, Perkin Transactions 2: Physical Organic  
 Chemistry (1972-1999) (1992), (9), 1425-9  
 CODEN: JCPKBH; ISSN: 0300-9580  
 DT Journal  
 LA English  
 AB Alkyl radicals generated in solution by UV photolysis add to C60 to form  
 adducts of the type RC60, whose EPR spectra are discussed. When R = CCl3,  
 CBr3, tert-Bu or 1-adamantyl, the spectrum is sufficiently powerful to  
 permit the detection of several <sup>13</sup>C satellites associated with the C60  
 component of the free radical. It is concluded from the intensities and  
 hyperfine interactions of these satellites that ca. 2/3 of the unpaired  
 spin population is located on the three carbon atoms ortho to that bearing  
 the incoming radical R. There is evidence from the temperature dependence of  
 the EPR spectra of certain RC60 radicals that they exist in equilibrium with  
 their dimer, RC60C60R. For R = iso-Pr, tert-Bu, 1-adamantyl and CCl3, the  
 enthalpy of dissociation is 35.5, 22.0, 21.6 and 17.1 kcal mol<sup>-1</sup> resp.  
 IT **140656-83-3P 140656-84-4P 140656-85-5P**  
 RL: PRP (Properties); FORM (Formation, nonpreparative); PREP (Preparation)  
 (formation and ESR of)  
 RN 140656-83-3 CAPLUS  
 CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 2-(phenylmethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



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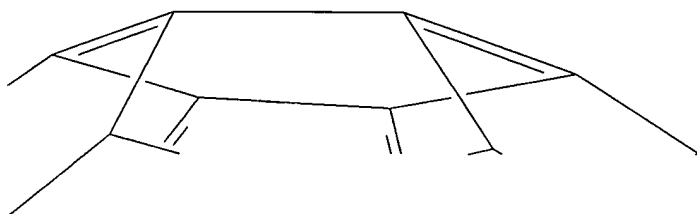
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

RN 140656-84-4 CAPLUS

CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 2-(phenylmethyl-13C)- (9CI) (CA INDEX  
NAME)

PAGE 1-A

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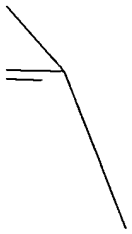
RN 140656-85-5 CAPLUS

CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 2-(phenyl-d5-methyl)- (9CI) (CA INDEX NAME)

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

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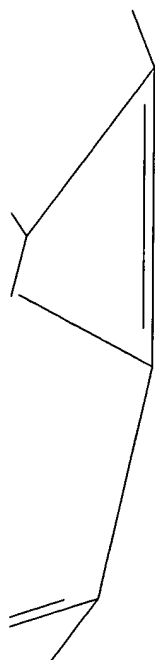




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PAGE 2-C



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PAGE 3-C

L5 ANSWER 39 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1992:204227 CAPLUS  
 DN 116:204227  
 TI ESR studies of the reaction of alkyl radicals with fullerene (C60)  
 AU Morton, J. R.; Preston, K. F.; Krusic, P. J.; Hill, S. A.; Wasserman, E.  
 CS Steacie Inst. Mol. Sci., Natl. Res. Counc. Canada, Ottawa, ON, K1A 0R9,  
 Can.  
 SO Journal of Physical Chemistry (1992), 96(9), 3576-8  
 CODEN: JPCHAX; ISSN: 0022-3654  
 DT Journal  
 LA English  
 AB Photolytically and thermally generated alkyl radicals (R• = tert-Bu,  
 1-adamantyl, iso-Pr, Et, and benzyl) react with C60 to form R-C60•  
 radical adducts which were identified by the proton and 13C hyperfine  
 interactions obtained from their ESR spectra. Consideration of the 13C  
 spectra shows that the unpaired electron in R-C60• is mostly confined  
 to 2 fused, 6-membered rings on the C60 surface, having the substituent R

at one of the points of fusion. Each half of the resulting radical structure of Cs symmetry can be compared with a cyclohexadienyl radical. Extensive delocalization of the unpaired electron over the C60 sphere is ruled out.

IT **140656-83-3P 140656-84-4P 140656-85-5P**

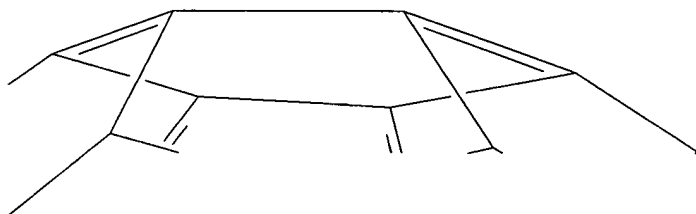
RL: PRP (Properties); PREP (Preparation)

(formation and ESR spectrum of, from reaction of fullerene with photolytically or thermally generated alkyl radicals)

RN 140656-83-3 CAPLUS

CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 2-(phenylmethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



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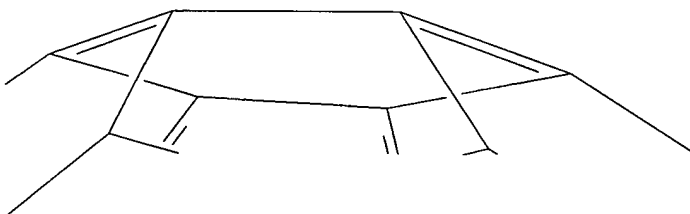
RN 140656-84-4 CAPLUS

CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 2-(phenylmethyl-13C)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



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RN 140656-85-5 CAPLUS

CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 2-(phenyl-d5-methyl)- (9CI) (CA INDEX NAME)

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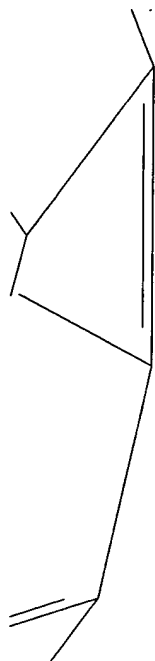
PAGE 1-C



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PAGE 2-C



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PAGE 3-C

L5 ANSWER 40 OF 40 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 1992:193587 CAPLUS  
 DN 116:193587  
 TI Radical reactions of C60  
 AU Krusic, P. J.; Wasserman, E.; Keizer, P. N.; Morton, J. R.; Preston, K. F.  
 CS E. I. du Pont de Nemours and Co., Wilmington, DE, 19880-0328, USA  
 SO Science (Washington, DC, United States) (1991), 254(5035),  
 1183-5  
 CODEN: SCIEAS; ISSN: 0036-8075  
 DT Journal  
 LA English  
 AB Photochem. generated benzyl radicals react with C60 producing radical and nonradical adducts RnC60 (R = C6H5CH2) with n = 1 to at least 15. The radical adducts with n = 3 and 5 are stable above 50° and have been identified by ESR spectroscopy as the allylic R3C60• and cyclopentadienyl R5C60• radicals. The unpaired electrons are highly localized on the C60 surface. The extraordinary stability of these

radicals can be attributed to the steric protection of the surface radical sites by the surrounding benzylsubstituents. Photochem. generated Me radicals also add readily C60. Mass spectrometric analyses show the formation of (CH<sub>3</sub>)<sub>n</sub>C<sub>60</sub> with n = 1 to at least 34.

IT **140700-29-4P**

RL: PREP (Preparation)  
(allylic, formation and ESR of)

RN 140700-29-4 CAPLUS

CN [5,6]Fulleren-C60-Ih-1(2H)-yl, 10,14-dihydro-2,10,14-tris(phenylmethyl)-  
(9CI) (CA INDEX NAME)

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

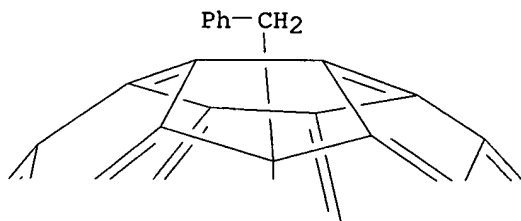
IT **139141-78-9P**

RL: PREP (Preparation)  
(cyclopentadienyl, formation and ESR of)

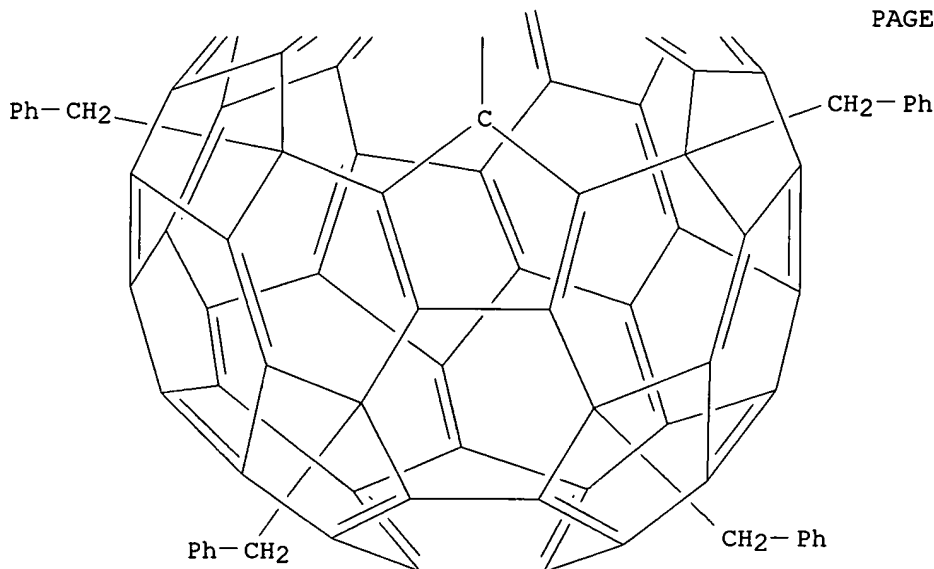
RN 139141-78-9 CAPLUS

CN [5,6]Fulleren-C60-Ih-1(9H)-yl, 6,12,15,18-tetrahydro-6,9,12,15,18-pentakis(phenylmethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A







=> s 14 not 15

L6 49 L4 NOT L5

=> dis 16 1-49 bib abs

L6 ANSWER 1 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2006:283633 CAPLUS

TI Titanium(III) Trisamidotriazacyclononane: Reactions with C60 and Radicals  
 AU Barroso, Sonia; Cui, Jinlan; Dias, Alberto R.; Duarte, M. Teresa;  
 Ferreira, Humberto; Henriques, Rui T.; Oliveira, M. Conceicao; Ascenso,  
 Jose R.; Martins, Ana M.

CS Centro de Quimica Estrutural, Instituto Superior Tecnico, Lisbon,  
 1049-001, Port.

SO Inorganic Chemistry (2006), 45(9), 3532-3537  
 CODEN: INOCAJ; ISSN: 0020-1669

PB American Chemical Society

DT Journal

LA English

AB The reaction of titanium trisamidotriazacyclononane,  $[\text{Ti}\{\text{N}(\text{Ph})\text{SiMe}_2\}_3\text{tacn}]$  (1), with C60 gave  $[\text{Ti}\{\text{N}(\text{Ph})\text{SiMe}_2\}_3\text{tacn}]\text{C}_{60}$  (2) in high yield. Treatment of 2 with  $\text{PhCH}_2\text{Br}$  gave  $[\text{Ti}\{\text{N}(\text{Ph})\text{SiMe}_2\}_3\text{tacn}]\text{Br}$  and the radical  $\text{PhCH}_2\text{C}_{60}$  (3). The reaction of  $\text{CH}_3\text{I}$  with 1 gives two products. One is  $[\text{Ti}\{\text{N}(\text{Ph})\text{SiMe}_2\}_3\text{tacn}]\text{I}$  (4), which results from the oxidation of 1 by an I radical. The other product, 5, resulting from a multistep reaction scheme that involves redox and nucleophilic reactions, presents an imido ligand formed by ligand rearrangement upon C-N bond cleavage. In solution, an exchange process that corresponds to a reversible 1,3-silyl shift between two Ti-bonded N atoms leads to isomers 5a and 5b. This equilibrium transforms an imido ( $\text{TiNPh}$ ) into an amido ligand ( $\text{Ti}\{\text{NPh}\}\text{SiMe}_2\text{CH}_2\text{Ph}$ ) with concomitant generation of an anionic moiety in the originally neutral triazacyclononane ring. In solution, either 5a or 5b displays addnl. fluxional processes that consist of its corresponding racemization processes.

RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2005:451357 CAPLUS  
DN 143:7512  
TI A preparation of octahydrophenanthrenecarboxylic acid hydrazide  
derivatives, useful as glucocorticoid receptor modulators  
IN Robinson, Ralph Pelton, Jr.; Kleinman, Edward Fox; Cheng, Hengmiao  
PA Pfizer Products Inc., USA  
SO PCT Int. Appl., 44 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005047254	A1	20050526	WO 2004-IB3671	20041108
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRAI US 2003-519937P	P	20031113		
OS MARPAT 143:7512				
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The invention relates to a preparation of octahydrophenanthrenecarboxylic acid hydrazide derivs. of formula I [wherein: R1 is 1 to 6 independent substituents; R2 is 1 or 2 independent substituents selected from H, alkyl optionally substituted with 1-3 halogens, alkynyl, or OH, etc.; R3 is heterocycle], useful as glucocorticoid receptor modulators. The invention compds. are useful in the treatment of obesity, diabetes, anxiety, or inflammatory diseases. For instance, octahydrophenanthrenecarboxylic acid hydrazide derivative II was prepared from naphthalene derivative III in 9 steps.

Preferred invention compds. showed ED50 less than 3  $\mu$ M.

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2005:441043 CAPLUS  
DN 143:115583  
TI Syntheses, Structure, and Derivatization of Potassium Complexes of Penta(organo)[60]fullerene-Monoanion, -Dianion, and -Trianion into Hepta- and Octa(organo)fullerenes  
AU Matsuo, Yutaka; Nakamura, Eiichi

CS Nakamura Functional Carbon Cluster Project ERATO, Japan Science and Technology Agency, Tokyo, 113-0033, Japan

SO Journal of the American Chemical Society (2005), 127(23), 8457-8466 . CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

LA English

OS CASREACT 143:115583

AB Two-electron reduction of penta(organo)[60]fullerenes C60Ar5H (Ar = Ph and biphenyl) by K/Hg amalgam afforded K complexes of the corresponding open-shell radical dianions  $[K^+(THF)_n]_2[C60Ar52-\bullet]$ . These compds. were characterized by UV-visible-near-IR and ESR spectroscopy in solution. Anaerobic crystallization of  $[K^+(THF)_n]_2[C60(biphenyl)52-\bullet]$  that exists largely as a monomer in solution gave black crystals of its dimer  $[K^+(THF)_3]_4[(biphenyl)5C60-C60(biphenyl)54-]$ , in which the two fullerene units are connected by a C-C single bond [1.577(11) Å] as determined by x-ray diffraction. Three-electron reduction of C60Ar5H with metallic K gave a black-green trianion  $[K^+(THF)_n]_3[C60Ar53-]$ . The reaction of the trianion with an alkyl halide RBr (R = PhCH<sub>2</sub> and Ph<sub>2</sub>CH) regioselectively afforded a hepta-organofullerene C60Ar5R<sub>2</sub>H, from which a K complex  $[K^+(THF)_n][C60(biphenyl)5(CH_2Ph)_2-]$  and a Pd complex  $Pd[C60(biphenyl)5(CH_2Ph)_2](\pi\text{-methallyl})$  as well as octa-organofullerene compds. C60(biphenyl)5(CH<sub>2</sub>Ph)<sub>3</sub>H<sub>2</sub> and Ru[C60(biphenyl)5(CH<sub>2</sub>Ph)<sub>3</sub>H]Cp were synthesized. These compds. possess dibenzo-fused corannulene  $\pi$ -electron conjugated systems and are luminescent.

RE.CNT 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2005:99334 CAPLUS

DN 142:170109

TI Antigluco corticoids for the treatment of catatonia

IN Belanoff, Joseph K.

PA Corcept Therapeutics, Inc., USA

SO PCT Int. Appl., 28 pp.  
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005009388	A2	20050203	WO 2004-US23761	20040723
	WO 2005009388	A3	20050616		
	W:				
	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW:				
	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2005080066	A1	20050414	US 2004-896143	20040720
	AU 2004259011	A1	20050203	AU 2004-259011	20040723
	CA 2532594	AA	20050203	CA 2004-2532594	20040723
	EP 1648469	A2	20060426	EP 2004-779017	20040723

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK

PRAI US 2003-489671P P 20030723  
WO 2004-US23761 W 20040723

AB The invention provides a method of ameliorating the symptoms of catatonia in a patient who is in need of treatment for catatonia. The method comprises administration of a therapeutically effective amount of a glucocorticoid receptor antagonist to the patient.

L6 ANSWER 5 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2005:99329 CAPLUS  
DN 142:170108  
TI Antiglucoctcoid therapy for the prevention of neurological damage in premature infants receiving glucocorticoid therapy  
IN Belanoff, Joseph K.  
PA Corcept Therapeutics, Inc., USA  
SO PCT Int. Appl., 25 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005009382	A2	20050203	WO 2004-US23592	20040722
	WO 2005009382	A3	20050929		
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
	RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	US 2005080061	A1	20050414	US 2004-896149	20040720
	AU 2004258992	A1	20050203	AU 2004-258992	20040722
	CA 2532415	AA	20050203	CA 2004-2532415	20040722
	EP 1648439	A2	20060426	EP 2004-757208	20040722
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR			
PRAI	US 2003-489601P	P	20030723		
	WO 2004-US23592	W	20040722		

AB This invention pertains to the discovery that agents which inhibit the binding of cortisol to its receptors can be used in methods for preventing neurol. damage associated with glucocorticoid therapy in ventilator-dependent low birth weight preterm infants. Mifepristone, a potent glucocorticoid receptor antagonist, can be used in these methods.

L6 ANSWER 6 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2004:1013677 CAPLUS  
DN 142:134293  
TI Manganese(III) acetate-mediated free radical reactions of [60]fullerene with  $\beta$ -dicarbonyl compounds  
AU Li, Changzhi; Zhang, Danwei; Zhang, Xiaotong; Wu, Shihui; Gao, Xiang  
CS Department of Chemistry, Fudan University, Shanghai, 200433, Peop. Rep. China

SO Organic & Biomolecular Chemistry (2004), 2(23), 3464-3469  
CODEN: OBCRAK; ISSN: 1477-0520

PB Royal Society of Chemistry

DT Journal

LA English

OS CASREACT 142:134293

AB [60]Fullerene reacted with various  $\beta$ -dicarbonyl compds. in the presence of  $\text{Mn}(\text{OAc})_3 \cdot 2\text{H}_2\text{O}$  to generate dihydrofuran-fused [60]fullerene derivs. or 1,4-bisadducts. Dihydrofuran-fused [60]fullerene derivs. could be formed by treatment of  $\alpha$ -unsubstituted  $\beta$ -diketones or  $\beta$ -ketoesters with [60]fullerene in refluxing chlorobenzene in the presence of  $\text{Mn}(\text{III})$ . Solvent-participated unsym. 1,4-bisadducts were obtained through the reaction of [60]fullerene with di-Me malonate or  $\alpha$ -substituted  $\beta$ -dicarbonyl compds. in toluene. A possible reaction mechanism for the formation of different fullerene derivs. is proposed.

RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2004:681540 CAPLUS

DN 141:185588

TI Methods for the treatment of postpartum psychosis with glucocorticoid receptor antagonists

IN Belanoff, Joseph K.

PA Corcept Therapeutics, Inc, USA

SO PCT Int. Appl., 27 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004069202	A2	20040819	WO 2004-US3183	20040204
	WO 2004069202	A3	20050106		
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI			
	RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	AU 2004208842	A1	20040819	AU 2004-208842	20040204
	CA 2514966	AA	20040819	CA 2004-2514966	20040204
	US 2004229855	A1	20041118	US 2004-772919	20040204
	EP 1599208	A2	20051130	EP 2004-708184	20040204
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
PRAI	US 2003-445284P	P	20030204		
	WO 2004-US3183	W	20040204		

AB This invention generally pertains to the field of psychiatry. In particular, this invention pertains to the discovery that agents which inhibit the binding of cortisol to its receptors can be used in methods for treating postpartum psychosis. Mifepristone, a potent specific glucocorticoid receptor antagonist, can be used in these methods. The invention also provides a kit for treating postpartum psychosis in a human including a glucocorticoid receptor antagonist and instructional material

teaching the indications, dosage and schedule of administration of the glucocorticoid receptor antagonist.

L6 ANSWER 8 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2004:450745 CAPLUS

DN 141:23730

TI Preparation of hydro(alkyl)fullerenes and their transition metal complexes, pentahydrofullarene transition metal complexes, and pentaalkylfullerenes

IN Nakamura, Eiichi; Togano, Motoki

PA Mitsubishi Chemical Corp., Japan

SO Jpn. Kokai Tokkyo Koho, 22 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	JP 2004155674	A2	20040603	JP 2002-320701	20021105
PRAI	JP 2002-320701		20021105		
GI					

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Hydro(alkyl)fullerenes  $C_xR_sH(5-s)H$  [I;  $C_x$  = fullerene skeleton;  $R$  = (C1-10 substituent-containing) alkyl, (C1-10 substituent-containing) aryl;  $x$  = even number

of  $\geq 60$ ;  $s = 0-4$ ] are prepared by treatment of fullerenes or fullerene-organic compound adducts  $C_xR_p$  (II) or  $C_xR_pH$  (III) ( $C_x$ ,  $R$ ,  $x$ ,  $s$  = same as above;  $p = 2, 4$ ;  $q = 1, 3$ ) with transition metal precursors and optional reducing agents in the presence of protonation agents.

Hydroalkylfullerene transition metal complexes  $C_xR_mH(5-m)ML_n$  (IV;  $C_x$ ,  $R$ ,  $x$  = same as I;  $M$  = transition metal;  $L$  = ligand;  $m = 1-4$ ;  $n = 0-5$ ) are prepared by treatment of II or III with transition metal precursors and optional reducing agents. Pentahydrofullerene transition metal complexes  $C_xH_5ML_n$  ( $C_x$ ,  $x$  = same as I;  $M$ ,  $L$ ,  $n$  = same as IV) are prepared by treatment of fullerenes with transition metal precursors and optional reducing agents. Pentaalkylfullerene metal complexes  $C_xR_mR'(5-m)ML_n$  [V;  $C_x$ ,  $x$ ,  $R$  = same as I;  $R'$  = (C1-10 substituent-containing) alkyl, (C1-10 substituent-containing) aryl;  $M$ ,  $L$ ,  $m$ ,  $n$  = same as IV] are prepared by

treatment

of  $C_xR_mH(5-m)ML_n$  ( $C_x$ ,  $R$ ,  $M$ ,  $L$ ,  $m$ ,  $n$  = same as V) with  $R'X$  ( $R'$  same as V;  $X$  = leaving group). Thus, C60 fullerene was treated with  $[FeCp(CO)_2]_2$  ( $Cp$  =  $\eta^5$ -cyclopentadienyl) to give 25% VI.

L6 ANSWER 9 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2004:447092 CAPLUS

DN 141:7284

TI Preparation of hydro(alkyl)fullerenes and their transition metal complexes, and pentahydrofullerene transition metal complexes

IN Nakamura, Eiichi; Togano, Motoki

PA Mitsubishi Chemical Corp., Japan

SO Jpn. Kokai Tokkyo Koho, 17 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2004155675	A2	20040603	JP 2002-320702	20021105
PRAI	JP 2002-320702		20021105		
OS	CASREACT 141:7284				
GI					

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Hydro(alkyl)fullerenes C<sub>x</sub>R<sub>p</sub>H(5-p)H [1; C<sub>x</sub> = fullerene skeleton; R = (C1-10 substituent-containing) alkyl, (C1-10 substituent-containing) aryl; x = even number

of  $\geq 60$ ; p = 0-4] having partial structures II (A = H, R; R = same as 1; P = H), hydroalkylfullerene transition metal complexes C<sub>x</sub>R<sub>m</sub>H(5-m)ML<sub>n</sub> (3; C<sub>x</sub>, R, x = same as 1; M = transition metal; L =  $\eta^1$ - or  $\eta^2$ -ligand; m = 1-4; n = 0-5) having partial structures IV (A = same as II; M, L, n = same as 3), and pentahydrofullerene transition metal complexes C<sub>x</sub>H<sub>5</sub>ML<sub>n</sub> (C<sub>x</sub>, x = same as 1; M, L, n = same as 3) having partial structures V (M, L, n = same as 3) are prepared. Thus, C<sub>60</sub> fullerene having partial structure II (A = H, P = CH<sub>2</sub>Ph) was treated with 9,10-dihydroanthracene and Re<sub>2</sub>(CO)<sub>10</sub> to give 42% C<sub>60</sub> fullerene having partial structure IV (one of A = CH<sub>2</sub>Ph, others of A = H, M = Re, L = CO, n = 3).

L6 ANSWER 10 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2004:412780 CAPLUS

DN 140:400079

TI Methods for treating gastroesophageal reflux disease with glucocorticoid receptor antagonists

IN Belanoff, Joseph K.

PA Corcept Therapeutics, Inc., USA

SO PCT Int. Appl., 27 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004041215	A2	20040521	WO 2003-US35341	20031105
	WO 2004041215	A3	20041104		
	W:				
	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				
	CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,				
	GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,				
	LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,				
	OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,				
	TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW:				
	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,				
	BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,				
	ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,				
	TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2504751	AA	20040521	CA 2003-2504751	20031105
	AU 2003291322	A1	20040607	AU 2003-291322	20031105
	US 2004132703	A1	20040708	US 2003-703069	20031105

US 2004167110 A1 20040826 US 2003-702950 20031105  
 EP 1567167 A2 20050831 EP 2003-768714 20031105  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK  
 JP 2006507311 T2 20060302 JP 2004-550523 20031105  
 PRAI US 2002-424199P P 20021105  
 WO 2003-US35341 W 20031105  
 AB This invention relates to the discovery that agents capable of inhibiting  
 the biol. action of the glucocorticoid receptor can be used in methods for  
 treating gastroesophageal reflux disease in a subject. The glucocorticoid  
 receptor antagonist is especially mifepristone.

L6 ANSWER 11 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2004:412779 CAPLUS  
 DN 140:400109  
 TI Methods using glucocorticoid receptor antagonists for treating migraine  
 IN Belanoff, Joseph K.  
 PA Corcept Therapeutics, Inc., USA  
 SO PCT Int. Appl., 30 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004041214	A2	20040521	WO 2003-US35328	20031105
WO 2004041214	A3	20041111		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,				
GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,				
LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,				
OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,				
TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,				
BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,				
ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,				
TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2504697	AA	20040521	CA 2003-2504697	20031105
AU 2003291314	A1	20040607	AU 2003-291314	20031105
US 2004132703	A1	20040708	US 2003-703069	20031105
US 2004167110	A1	20040826	US 2003-702950	20031105
EP 1581234	A2	20051005	EP 2003-768706	20031105
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006508951	T2	20060316	JP 2004-550521	20031105
US 2006052354	A1	20060309	US 2005-533146	20050427
PRAI US 2002-424199P	P	20021105		
WO 2003-US35328	W	20031105		
AB The invention relates to the discovery that agents capable of inhibiting the biol. action of the glucocorticoid receptor can be used in methods for treating migraine in a subject.				

L6 ANSWER 12 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2004:383047 CAPLUS  
 DN 140:385394  
 TI Discovery of potent, non-steroidal and highly selective glucocorticoid  
 receptor antagonists with anti-obesity activity  
 AU Morgan, Bradley P.; Liu, Kevin K.-C.; Dalvie, Deepak K.; Swick, Andrew G.;



Hargrove, Diane M.; Wilson, Theresa C.; LaFlamme, Janet A.; Moynihan, Melinda S.; Rushing, Margaret A.; Woodworth, Graeme F.; Li, Jisong; Trilles, Richard V.; Yang, Xiaojing; Harper, Kenneth W.; Carroll, Richard S.; Martin, Kelly A.; Nardone, Nancy A.; O'Donnell, John P.; Faletto, Michael B.; Vage, Chandravathi; Soliman, Victor

CS Pfizer Global Research and Development, Pfizer Inc., Groton, CT, 06340, USA

SO Letters in Drug Design & Discovery (2004), 1(1), 1-5  
CODEN: LDDDAW; ISSN: 1570-1808

PB Bentham Science Publishers Ltd.

DT Journal; General Review

LA English

AB A review. To thwart phase II metabolism, Structure-Activity-Relationship (SAR) studies around the phenol of the potent glucocorticoid receptor (GR) antagonists CP-394531 and CP-409069 were examined. The discovery of the potent; selective, nonsteroidal GR antagonist (CP-472555) with anti-GR and anti-obesity activity in animal models is described.

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 13 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2004:274878 CAPLUS

DN 141:54056

TI Selective addition to [60]fullerene of two different radicals generated from Mn(III)-based radical reaction

AU Wang, Guan-Wu; Zhang, Ting-Hu; Cheng, Xin; Wang, Fan

CS Department of Chemistry, University of Science and Technology of China, Hefei, 230026, Peop. Rep. China

SO Organic & Biomolecular Chemistry (2004), 2(8), 1160-1163  
CODEN: OBCRAK; ISSN: 1477-0520

PB Royal Society of Chemistry

DT Journal

LA English

OS CASREACT 141:54056

AB Reaction of [60]fullerene in PhMe with  $\text{RCH}(\text{CO}_2\text{Et})_2$  [ $\text{R} = \text{Me}, \text{Et}, \text{Br}$ ]  $\text{CH}(\text{CO}_2\text{Et})_3$ , and  $\text{NCCH}_2\text{CO}_2\text{Et}$  in the presence of  $\text{Mn}(\text{OAc})_3 \cdot 2\text{H}_2\text{O}$  afforded benzyl-substituted unsym. 1,4-adducts. Dibenzylated 1,4-adduct and a methanofullerene 6 were also obtained in the case of  $\text{CH}(\text{CO}_2\text{Et})_3$  and  $\text{NCCH}_2\text{CO}_2\text{Et}$ , resp. A possible reaction mechanism for the formation of the 1,4-adducts is proposed.

RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 14 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2004:141753 CAPLUS

DN 140:339056

TI Methodology for the Preparation of Cl-Monoalkylated 1,2-Dihydro[C70] Derivatives: Formation of the "Other" Regioisomer

AU Wang, Zhongwen; Meier, Mark S.

CS Department of Chemistry, University of Kentucky, Lexington, KY, 40506-0055, USA

SO Journal of Organic Chemistry (2004), 69(6), 2178-2180  
CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

OS CASREACT 140:339056

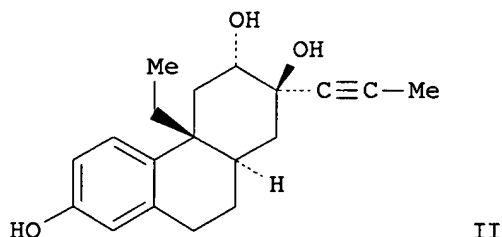
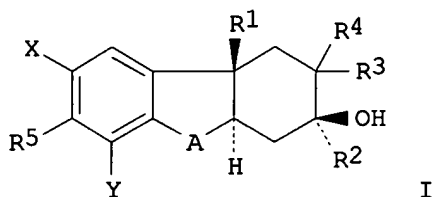
AB Deprotonation of 1,2-C70H2 with  $\text{Bu}_4\text{N}^+ \text{OH}^-$ , followed by alkylation with Me

bromoacetate, results in formation of a C(1)-monoalkylated 1,2-dihydro-C70 derivative. The position of the alkyl group (C-1) was established by NMR spectroscopy and comparison with literature spectra of C(2)-monoalkylated analogs. Presumably, C(1)-alkylation is the major process due to selective deprotonation of 1,2-C70H2 at C-1. Substitution of benzyl bromide for Me bromoacetate results in rapid dialkylation, unless the amount of base is carefully controlled, in which case C(1)-monobenzylation is the major process. This methodol. for alkylation at C-1 is complimentary to methods for the C(2)-monoalkylation of C70 with Zn and Me bromoacetate.

RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 15 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2004:41424 CAPLUS  
DN 140:111136  
TI Preparation of octahydrophenanthrenols as glucocorticoid receptor  
modulators for treatment of inflammatory conditions  
IN Chantigny, Yves Andre; Kleinman, Edward Fox; Robinson, Ralph Pelton, Jr.  
PA Pfizer Products Inc., USA  
SO PCT Int. Appl., 143 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004005229	A1	20040115	WO 2003-IB2941	20030625
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2491994	AA	20040115	CA 2003-2491994	20030625
	AU 2003281355	A1	20040123	AU 2003-281355	20030625
	EP 1521733	A1	20050413	EP 2003-740911	20030625
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	BR 2003012575	A	20050503	BR 2003-12575	20030625
	JP 2005532389	T2	20051027	JP 2004-519100	20030625
	US 2004138262	A1	20040715	US 2003-615126	20030708
PRAI	US 2002-394425P	P	20020708		
	WO 2003-IB2941	W	20030625		
OS	MARPAT 140:111136				
GI					



AB Title compds. I [wherein A = CR<sub>6</sub>R<sub>7</sub>CR<sub>8</sub>R<sub>9</sub>, COCR<sub>10</sub>R<sub>11</sub>, or CR<sub>12</sub>=CR<sub>13</sub>; X and Y = independently H, F, Cl, Br, or alkyl; R<sub>1</sub> = alkyl, alkenyl, or (un)substituted benzyl; R<sub>2</sub> = (un)substituted (cyclo)alkyl(alkyl), alkenyl, alkynyl, (hetero)aryl(alkyl), or heterocyclyl(alkyl); R<sub>3</sub> = H or (un)substituted (cyclo)alkyl, alkenyl, alkynyl, heterocyclyl, or (hetero)aryl; R<sub>4</sub> = OH or NR<sub>14</sub>R<sub>15</sub>; R<sub>5</sub> = H, halo, OH, CN, or (un)substituted (cyclo)alkyl(oxy), alkenyl, alkynyl, (hetero)aryl(oxy), heterocyclyl(oxy), carbamoyl, sulfamoyl, acyl(oxy), etc.; R<sub>6</sub>-R<sub>9</sub> = independently H, alkyl, F, or OH; R<sub>10</sub> and R<sub>11</sub> = independently H or alkyl; R<sub>12</sub> and R<sub>13</sub> = independently H, F, or alkyl; R<sub>14</sub> and R<sub>15</sub> = independently H or alkyl; and pharmaceutically acceptable salts thereof] were prepared as glucocorticoid receptor agonists (no data). For example, (3S,4aR,10aR)-3-bromo-4a-ethyl-7-hydroxy-3,4,4a,9,10,10a-hexahydro-1H-phenanthren-2-one (multi-step preparation given) was treated with NaOH in DMF and H<sub>2</sub>O followed by 0.2M HCl to give a 2:1 mixture of the 2-keto-3-hydroxy and 2-hydroxy-3-keto derivs. The 2-keto enriched compound (9:1 ratio of 2-keto to 3-keto derivative) was alkylated with propyne in THF using BuLi in hexane to afford II (25%). Bioassays for glucocorticoid receptor modulation and antiinflammatory response are described, but no specific data are provided. Thus, I and their pharmaceutical compns., salts, and prodrugs are useful in the treatment of certain inflammatory disorders, endocrine disorders, collagen diseases, dermatol. diseases, allergic states, ophthalmic diseases, respiratory diseases, hematol. disorders, neoplastic diseases, edematous states, and gastrointestinal diseases (no data).

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 16 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2004:41222 CAPLUS  
DN 140:87727  
TI Methods using a glucocorticoid receptor antagonist for treating psychosis associated with interferon- $\alpha$  therapy  
IN Belanoff, Joseph K.  
PA Corcept Therapeutics, Inc., USA  
SO PCT Int. Appl., 36 pp.  
CODEN: PIXXD2  
DT Patent

LA English  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004004653	A2	20040115	WO 2003-US21245	20030702
	WO 2004004653	A3	20040826		
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	CA 2491296	AA	20040115	CA 2003-2491296	20030702
	AU 2003269898	A1	20040123	AU 2003-269898	20030702
	EP 1534299	A2	20050601	EP 2003-751785	20030702
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
	CN 1665515	A	20050907	CN 2003-815811	20030702
	JP 2005535664	T2	20051124	JP 2004-519990	20030702
	US 2006063748	A1	20060323	US 2004-519008	20041221
PRAI	US 2002-393660P	P	20020702		
	WO 2003-US21245	W	20030702		
AB	The invention discloses methods using a glucocorticoid receptor antagonist for the treatment of psychosis associated with interferon- $\alpha$ therapy. The invention further discloses kits for the treatment of Hepatitis C in a patient.				

L6 ANSWER 17 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2003:844743 CAPLUS

DN 140:59737

TI Synthesis of Ferrocene/Hydrofullerene Hybrid and Functionalized Bucky Ferrocenes

AU Toganoh, Motoki; Matsuo, Yutaka; Nakamura, Eiichi

CS Department of Chemistry, The University of Tokyo, Bunkyo, Tokyo, 113-0033, Japan

SO Journal of the American Chemical Society (2003), 125(46), 13974-13975  
CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

LA English

OS CASREACT 140:59737

AB Hydroferration reaction of [60]fullerene or its derivs., C<sub>60</sub>(CH<sub>2</sub>Ph)<sub>2</sub> and C<sub>60</sub>(CH<sub>2</sub>Ph)<sub>2</sub>PhH, with [Fe(C<sub>5</sub>H<sub>5</sub>)(CO)<sub>2</sub>]<sub>2</sub> gives regioselectively a ferrocene/hydrofullerene hybrid, which upon treatment with Bu<sub>4</sub>NOH and an alkyl halide affords the corresponding alkylated bucky ferrocene, e.g., Fe(C<sub>60</sub>H<sub>5</sub>)(C<sub>5</sub>H<sub>5</sub>), again regioselectivity via an anion of the ferrocene. These alkylation conditions were applied to the rhenium analog to afford, e.g., Re[C<sub>60</sub>(CH<sub>2</sub>Ph)<sub>4</sub>Ph](CO)<sub>3</sub> in 48% yield..

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 18 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2003:827349 CAPLUS

DN 140:59751

TI Synthesis and catalytic activity of rhodium diene complexes bearing indenyl-type fullerene  $\eta^5$ -ligand  
 AU Toganoh, Motoki; Matsuo, Yutaka; Nakamura, Eiichi  
 CS Department of Chemistry, The University of Tokyo, Hongo, Tokyo, 7-3-1, Japan  
 SO Journal of Organometallic Chemistry (2003), 683(2), 295-300  
 CODEN: JORCAI; ISSN: 0022-328X  
 PB Elsevier Science B.V.  
 DT Journal  
 LA English  
 OS CASREACT 140:59751  
 AB Rh  $\eta^5$ -complexes bearing an indenyl-type fullerene ligand, Rh[C60(PhCH2)2Ph](cod) (2), Rh[C60(PhCH2)2Ph](nbd) (3) and Rh(C70Ph3)(cod) (4), were synthesized from the corresponding fullerene tri-adducts in 93-96% yields. X-ray crystallog. anal. of 4 indicated that the structure of 4 is similar to that of Rh(Ind)(cod). The Rh complex 2 catalyzes alkyne trimerization reactions and hydroboration reactions.  
 RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 19 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2003:683501 CAPLUS  
 DN 140:128146  
 TI Mixed bis-functionalization of fullerene C60 from C602- anion  
 AU Cheng, Fuyong; Allard, Emmanuel; Chopin, Stephanie; Delaunay, Jacques; Cousseau, Jack  
 CS Laboratoire d'Ingenierie Moleculaire et Materiaux Organiques, UMR CNRS 6501, Universite d'Angers, Angers, 49045, Fr.  
 SO Proceedings - Electrochemical Society (2002), 2002-12(Fullerenes--Volume 12: The Exciting World of Nanocages and Nanotubes), 188-192  
 CODEN: PESODO; ISSN: 0161-6374  
 PB Electrochemical Society  
 DT Journal  
 LA English  
 OS CASREACT 140:128146  
 AB Mixed adducts bis-functionalization of fullerene can be derived from C602- anion. In particular functionalized dihydrofullerenes C60HR are thus obtained, and can be used for obtaining various bis-functionalization of fullerene derivs.  
 RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 20 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2003:655961 CAPLUS  
 DN 139:323635  
 TI Rhenium-templated regioselective polyhydrogenation reaction of [60]fullerene  
 AU Toganoh, Motoki; Matsuo, Yutaka; Nakamura, Eiichi  
 CS Department of Chemistry, The University of Tokyo, Tokyo, 113-0033, Japan  
 SO Angewandte Chemie, International Edition (2003), 42(30), 3530-3532  
 CODEN: ACIEF5; ISSN: 1433-7851  
 PB Wiley-VCH Verlag GmbH & Co. KGaA  
 DT Journal  
 LA English  
 OS CASREACT 139:323635  
 AB Rhenium-templated transfer hydrogenation from 9,10-dihydroanthracene (DHA) to [60]fullerene or its derivs. in water at 160° gave a 60% yield of cyclopentadiene-incorporated fullerene analog, e.g.,

C60(H)3(PhCH2)2(Ph) (2), which can be converted into the corresponding metal complexes. E.g., 2 reacts with {Fe(C5H5)(CO)2}2/PhCN at 160° to give a 28% yield of (C5H5)Fe[C60(H)3(PhCH2)2(Ph)].

RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 21 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2003:610236 CAPLUS

DN 139:154927

TI Pharmaceutical compositions of amorphous dispersions of drugs and lipophilic microphase-forming materials

IN Perlman, Michael Ellis; Shanker, Ravi Mysore; Babcock, Walter Christian; Friesen, Dwayne Thomas; Rabenstein, Mark David; Smithey, Daniel Tod

PA Pfizer Products Inc., USA

SO PCT Int. Appl., 89 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003063833	A1	20030807	WO 2003-IB335	20030128
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2474838	AA	20030807	CA 2003-2474838	20030128
	EP 1469832	A1	20041027	EP 2003-700435	20030128
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	BR 2003007344	A	20041214	BR 2003-7344	20030128
	JP 2005523262	T2	20050804	JP 2003-563527	20030128
	US 2003228358	A1	20031211	US 2003-355747	20030131
PRAI	US 2002-354081P	P	20020201		
	WO 2003-IB335	W	20030128		

AB A pharmaceutical composition comprises a solid amorphous dispersion comprising a low-solubility drug and a concentration-enhancing polymer and a lipophilic microphase-forming material. Alternatively, a solid amorphous dispersion comprising a low-solubility drug and a concentration-enhancing polymer is co-administered with a lipophilic microphase-forming material to an in vivo use environment. A spray solution was formed containing 2.5 wt% drug, 7.5 wt% HPMCAS-MF, and 90% acetone. The solution was spray-dried by directing a 2-fluid external-mix spray nozzle at 2.7 bar with a feed rate of 190 g/min into the stainless-steel chamber of a spray-dryer, by using nitrogen as the drying gas, maintained at a temperature of 137° at the inlet; the drying gas and evaporated solvent exited the drier at 49°. The resulting solid amorphous dispersion was collected and then dried in a solvent tray-drier by spreading the spray-dried particles onto polyethylene-lined trays to a depth of not more than 1 cm and then drying them at 40° for 25 h. After drying, dispersion 1 contained 25 wt% drug.

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD

## ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 22 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2003:534830 CAPLUS  
 DN 140:59390  
 TI Regioselective synthesis of [60]fullerene  $\eta^5$ -indenide R3C60- and  
 $\eta^5$ -cyclopentadienide R5C60- bearing different R groups  
 AU Toganoh, Motoki; Suzuki, Kazuhiro; Udagawa, Rie; Hirai, Atsushi; Sawamura,  
 Masaya; Nakamura, Eiichi  
 CS Department of Chemistry, The University of Tokyo, Bunkyo-ku, Japan  
 SO Organic & Biomolecular Chemistry (2003), 1(14), 2604-2611  
 CODEN: OBCRAK; ISSN: 1477-0520  
 PB Royal Society of Chemistry  
 DT Journal  
 LA English  
 OS CASREACT 140:59390  
 AB Treatment of a 1,7-diorgano[60]fullerene with Grignard reagents or  
 organocopper reagents affords a [60]fullerene indenide or a [60]fullerene  
 cyclopentadienide regioselectively in good to excellent yields. These  
 reactions gave an insight into the reaction mechanism of the organocopper  
 penta-addition reaction of [60]fullerene, giving [60]fullerene  
 cyclopentadienide in quant. yield.  
 RE.CNT 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 23 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2003:531546 CAPLUS  
 DN 139:108747  
 TI Fullerene-containing dye and application such as optical recording  
 materials, color composition for color filter, ink thereof  
 IN Saito, Yasunori; Tsukahara, Hiroshi; Ogiso, Akira; Misawa, Tsutayoshi  
 PA Mitsui Chemicals, Inc., Japan; Yamamoto Chemicals Inc.  
 SO Jpn. Kokai Tokkyo Koho, 41 pp.  
 CODEN: JKXXAF  
 DT Patent  
 LA Japanese  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
PI	JP 2003196881	A2	20030711	JP 2002-256809	20020902
PRAI	JP 2001-265981	A	20010903		
AB	The invention relates to a fullerene dye disposed in an organic dye layer as an optical recoding layer on a substrate. The dye provides the good recording/reading characteristic using 300-500 nm light.				

L6 ANSWER 24 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2003:394587 CAPLUS  
 DN 139:117205  
 TI C602- Chemistry: C60 Adducts Bearing Two Ester, Carbonyl, or Alcohol  
 Groups  
 AU Allard, Emmanuel; Delaunay, Jacques; Cousseau, Jack  
 CS Laboratoire D'Ingenierie Moleculaire et Materiaux Organiques, UMR CNRS  
 6501, Universite d'Angers, Angers, F-49045, Fr.  
 SO Organic Letters (2003), 5(13), 2239-2242  
 CODEN: ORLEF7; ISSN: 1523-7060  
 PB American Chemical Society  
 DT Journal  
 LA English

OS CASREACT 139:117205

AB Reactions of activated halo compds. XCH<sub>2</sub>-A (X = Br, I; A = ester, ketone) with C<sub>60</sub><sup>2-</sup> anion give rise to C<sub>60</sub>(CH<sub>2</sub>-A)<sub>2</sub> adducts (major products) along with unexpected methanofullerenes C<sub>60</sub>>CH-A and monosubstituted dihydrofullerenes C<sub>60</sub>(H)(CH<sub>2</sub>-A) (minor products). Methanofullerenes come from side reactions with X<sub>2</sub>CH-A traces.

RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 25 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2003:318751 CAPLUS

DN 139:164611

TI New, scalable route for the synthesis of a trans-fused hexahydro-1H-phenanthren-2-one from a conjugated tetrahydro-3H-phenanthren-2-one

AU Morgan, Bradley P.; Trilles, Richard V.; Woodworth, Graeme F.

CS Pfizer Global Research and Development, Pfizer Inc., Groton, CT, 06371, USA

SO Synthetic Communications (2003), 33(6), 915-920

CODEN: SYNCAV; ISSN: 0039-7911

PB Marcel Dekker, Inc.

DT Journal

LA English

OS CASREACT 139:164611

AB A three-step, readily scalable route for the conversion of a ring-conjugated tetrahydro-3H-phenanthren-2-one to a trans-fused hexahydro-1H-phenanthren-2-one is described. The key step is the hydrogenation of a double bond using a nearby ketal moiety to assist in the stereoselective delivery of the hydrogen.

RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 26 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2003:235760 CAPLUS

DN 138:385156

TI Monoalkylation of C<sub>60</sub> and C<sub>70</sub> with Zn and Active Alkyl Bromides

AU Wang, Zhongwen; Meier, Mark S.

CS Center for Advanced Carbon Materials and Department of Chemistry, University of Kentucky, Lexington, KY, 40506-0055, USA

SO Journal of Organic Chemistry (2003), 68(8), 3043-3048

CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

OS CASREACT 138:385156

AB A convenient and simple solution-phase electron-transfer reaction of C<sub>60</sub> with zinc and  $\alpha$ -bromoacetonitrile,  $\alpha$ -bromoacetates, allyl bromide, benzyl bromide and  $\alpha$ -bromo ketones in DMF gives different types of monoalkylated C<sub>60</sub> derivs. When this method is employed with C<sub>70</sub>, 2-carbomethoxymethyl-1,2-dihydro[70]fullerene is produced as one of the two 1,2-monoalkylated C<sub>70</sub> isomers, together with the first 5,6-monoalkylated C<sub>70</sub> derivative

RE.CNT 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 27 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2003:202422 CAPLUS

DN 138:232194



TI Methods for inhibiting cognitive deterioration in adults with Down's syndrome with glucocorticoid receptor blockade  
 IN Belanoff, Joseph K.  
 PA Corcept Therapeutics, Inc., USA  
 SO PCT Int. Appl., 36 pp.  
 CODEN: PIXXD2

DT Patent  
 LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003020216	A1	20030313	WO 2002-US27576	20020827
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2459033	AA	20030313	CA 2002-2459033	20020827
	EP 1432379	A1	20040630	EP 2002-770441	20020827
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
	CN 1556708	A	20041222	CN 2002-818608	20020827
	JP 2005501882	T2	20050120	JP 2003-524530	20020827
	US 2003064974	A1	20030403	US 2002-230575	20020828
	ZA 2004001754	A	20050303	ZA 2004-1754	20040303
	NO 2004001338	A	20040528	NO 2004-1338	20040331
PRAI	US 2001-316653P	P	20010831		
	WO 2002-US27576	W	20020827		

AB This invention generally pertains to the field of psychiatry. In particular, this invention pertains to the discovery that agents capable of inhibiting the binding of cortisol to its receptors can be used in methods for preventing or reversing cognitive deterioration in adults with Down's syndrome. Mifepristone, a potent specific glucocorticoid receptor antagonist, can be used in these methods. The invention also provides a kit for preventing or reversing cognitive deterioration in a DS patient including a glucocorticoid receptor antagonist and instructional material teaching the indications, dosage and schedule of administration of the glucocorticoid receptor antagonist.

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 28 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2003:49356 CAPLUS  
 DN 139:85110  
 TI Easy access to unprecedented mixed functionalized dihydrofullerenes C60RH and C60RR': the C602- anion route  
 AU Allard, Emmanuel; Cheng, Fuyong; Chopin, Stephanie; Delaunay, Jacques; Rondeau, David; Cousseau, Jack  
 CS Laboratoire IMMO (CNRS UMR 6501), Faculte des Sciences, Universite d'Angers, Angers, F-49045, Fr.  
 SO New Journal of Chemistry (2003), 27(2), 188-192  
 CODEN: NJCHE5; ISSN: 1144-0546  
 PB Royal Society of Chemistry

DT Journal  
 LA English  
 OS CASREACT 139:85110  
 AB Functionalized mixed dihydrofullerenes C60RH and C60RR' are easily obtained from reactions between C602- anion and halo derivs. RX and R'X. The key step consists of the selective reaction of the intermediate [C60R]- ion, as soon as it is formed, with either CF3CO2H or R'X. This process is made possible thanks to the very fast single electron transfer reaction between C602- and RX. Functionalized dihydrofullerenes C60RH thus prepared are also shown to be very good starting compds. for obtaining various C60RR' derivs.  
 RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 29 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN  
 AN 2003:5750 CAPLUS  
 DN 138:78446  
 TI Pharmaceutical compositions containing polymer and drug assemblies  
 IN Babcock, Walter Christian; Crew, Marshall David; Friesen, Dwayne Thomas; Rabenstein, Mark David; Smithey, Daniel Tod; Shanker, Ravi Mysore  
 PA Pfizer Products Inc., USA  
 SO PCT Int. Appl., 257 pp.  
 CODEN: PIXXD2

DT Patent  
 LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003000226	A2	20030103	WO 2002-IB2256	20020617
	WO 2003000226	A3	20031023		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2450748	AA	20030103	CA 2002-2450748	20020617
	US 2003170309	A1	20030911	US 2002-173945	20020617
	EP 1401399	A2	20040331	EP 2002-735849	20020617
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	BR 2002011028	A	20040615	BR 2002-11028	20020617
	JP 2004534811	T2	20041118	JP 2003-506873	20020617
PRAI	US 2001-300259P	P	20010622		
	WO 2002-IB2256	W	20020617		

AB Solns. containing polymer/drug assemblies of a low-solubility drug and an amphiphilic polymer are disclosed. In addition, solid aggregated polymer/drug assemblies are disclosed comprising a low-solubility drug and polymer. For example, amorphous solid dispersions of the low-solubility drug 5-chloro-1H-indole-2-carboxylic acid [(1S)-benzyl-3-((3R,4S)-dihydroxypyrroldin-1-yl)-(2R)-hydroxy-3-oxypropyl]amide and the amphiphilic polymer hydroxypropyl Me cellulose acetate succinate were prepared. When no drug was present, small particles about 10-20 nm in size were present due to aggregation of the polymer (HPMCAS-MF) with itself,

likely as a result of its amphiphilicity, which renders the polymer only sparingly water soluble. For solns. containing drug solid dispersions, particles were present with an average size of about 80 nm. This demonstrates the formation of polymer/drug assemblies in solution.

L6 ANSWER 30 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2002:524034 CAPLUS

DN 137:232437

TI Alkylation of Dihydrofullerenes

AU Meier, Mark S.; Bergosh, Robert G.; Gallagher, Megan E.; Spielmann, H. Peter; Wang, Zhongwen

CS Center for Advanced Carbon Materials and Department of Chemistry and Department of Molecular and Cellular Biochemistry, University of Kentucky, Lexington, KY, 40506-0055, USA

SO Journal of Organic Chemistry (2002), 67(17), 5946-5952

CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

OS CASREACT 137:232437

AB The fulleride dianions C60<sup>2-</sup> and C70<sup>2-</sup> were generated by deprotonation of the hydrogenated fullerenes, 1,2-C60H2 and 1,2-C70H2. These anions were prepared in the presence of a variety of alkylating agents and mono- or dialkylated products were obtained. Alkylation was not successful with sulfonate ester alkylating agents. Deprotonation of monoalkylated compds., followed by a second alkylation with a different alkylating agent, produced heterodiallylated compds. The monoalkylated material was invariably the 1,2-isomers, while the dialkylated materials were generally 1,4-isomers, although some 1,2-isomer was observed in the C70 product. The major product from alkylation of C70<sup>2-</sup> was the 7,23-isomer, a structure where the alkylation took place near the equator of the fullerene cage, rather than at the more strained carbons near the poles.

RE.CNT 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 31 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2002:348359 CAPLUS

DN 137:88411

TI Discovery of Potent, Nonsteroidal, and Highly Selective Glucocorticoid Receptor Antagonists

AU Morgan, Bradley P.; Swick, Andrew G.; Hargrove, Diane M.; LaFlamme, Janet A.; Moynihan, Melinda S.; Carroll, Richard S.; Martin, Kelly A.; Lee, Eunsun; Decosta, Debra; Bordner, Jon

CS Pfizer Global Research and Development, Pfizer Inc., Groton, CT, 06371, USA

SO Journal of Medicinal Chemistry (2002), 45(12), 2417-2424

CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

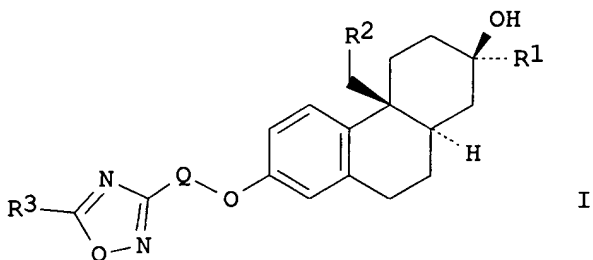
LA English

AB An approach to the computer-assisted, pharmacophore design of nonsteroidal templates for the glucocorticoid receptor (GR) that contained an element of pseudo-C2 symmetry was developed. The enantiomer of the initial design, and not the designed mol., showed the desired ligand binding to the GR. The pseudo-C2 symmetry of the template allowed for rapid improvements in GR activity resulting in potent, selective, nonsteroidal GR antagonists, CP-394531 and CP-409069.

RE.CNT 71 THERE ARE 71 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 32 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2002:330268 CAPLUS  
DN 136:340682  
TI Preparation of oxadiazolylalkoxyoctahydrophenanthrenes as glucocorticoid  
receptor modulators  
IN Liu, Kevin Kun-Chin; Morgan, Bradley P.; Robinson, Ralph Pelton  
PA Pfizer Products Inc., USA  
SO Eur. Pat. Appl., 39 pp.  
CODEN: EPXXDW  
DT Patent  
LA English  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1201660	A1	20020502	EP 2001-308789	20011016
	EP 1201660	B1	20050831		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	AT 303369	E	20050915	AT 2001-308789	20011016
	ES 2246292	T3	20060216	ES 2001-1308789	20011016
	CA 2360313	AA	20020430	CA 2001-2360313	20011026
	US 2004014741	A1	20040122	US 2001-12274	20011026
	US 6852719	B2	20050208		
	JP 2002193955	A2	20020710	JP 2001-330283	20011029
	BR 2001004834	A	20020820	BR 2001-4834	20011029
PRAI	US 2000-244302P	P	20001030		
OS	MARPAT 136:340682				
GI					



AB Title compds. [I; R1 = alkyl, trifluoroalkyl, C.tplbond.CMe, C.tplbond.CCl, C.tplbond.CCF3, CF3, etc.; R2 = alkyl, alkenyl, (substituted) Ph; R3 = alkyl, amino, aminoalkyl, heterocyclyl, heterocyclylalkyl; Q = (CH<sub>2</sub>)<sub>n</sub>; n = 1-3; with provisos], were prepared for treatment of obesity, diabetes, inflammation, anxiety, depression, and neurodegeneration (no data). Thus, ethanimidamide, N-hydroxy-2-[[4b,5,6,7,8,8a,9,10-octahydro-7-hydroxy-4b-(phenylmethyl)-7-(trifluoromethyl)-2-phenanthrenyl]oxy]- (preparation given) and NaH in THF were heated at 60° for 20 min. The solution was cooled to room temperature and ethyl-N,N-dimethylglycine was added. The resultant mixture was heated to reflux for 1 h to give 57% 2-phenanthrenol, 7-[[5-[(dimethylamino)methyl]-1,2,4-oxadiazol-3-yl]methoxy]-1,2,3,4,4a,9,10,10a-octahydro-4a-(phenylmethyl)-2-(trifluoromethyl)-, [2R-(2 $\alpha$ ,4 $\alpha$ ,10 $\alpha$ )]].

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

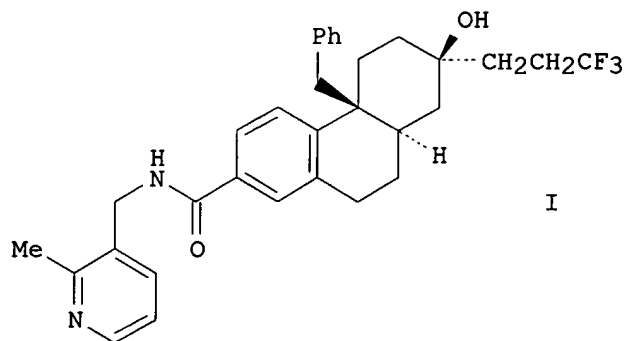
L6 ANSWER 33 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2002:330265 CAPLUS  
DN 136:340594  
TI Preparation of 4b(S)-benzyl-7(S)-hydroxy-7-(3,3,3-trifluoropropyl)-  
4b,5,6,7,8,8a(R),9,10-octahydrophenanthrene-2-carboxylic acid  
(2-methylpyridin-3-ylmethyl)amide via an amidation reaction using  
carbonyldiimidazole.

IN Murry, Jerry Anthony; White, Timothy Donald  
PA Pfizer Products Inc., USA  
SO Eur. Pat. Appl., 53 pp.  
CODEN: EPXXDW

DT Patent  
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1201655	A2	20020502	EP 2001-309057	20011025
	EP 1201655	A3	20020626		
	EP 1201655	B1	20050907		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	US 2002087005	A1	20020704	US 2001-8619	20011022
	US 6570020	B2	20030527		
	CA 2360024	AA	20020427	CA 2001-2360024	20011025
	CA 2539147	AA	20020427	CA 2001-2539147	20011025
	ZA 2001008797	A	20030425	ZA 2001-8797	20011025
	AT 303992	E	20050915	AT 2001-309057	20011025
	ES 2246293	T3	20060216	ES 2001-1309057	20011025
	AU 784269	B2	20060302	AU 2001-83622	20011025
	CN 1356319	A	20020703	CN 2001-135596	20011026
	JP 2002193937	A2	20020710	JP 2001-329529	20011026
	CN 1680243	A	20051012	CN 2005-10004526	20011026
	BR 2001004836	A	20021015	BR 2001-4836	20011029
	RU 2219170	C2	20031220	RU 2001-131115	20011119
	US 2003120081	A1	20030626	US 2002-271309	20021015
	US 6727392	B2	20040427		
PRAI	US 2000-243873P	P	20001027		
	US 2001-8619	B3	20011022		
	CA 2001-2360024	A3	20011025		
	CN 2001-135596	A3	20011026		
OS	CASREACT 136:340594				
GI					



AB Title compound (I) was prepared via reaction of 4b(S)-Benzyl-7(S)-hydroxy-7-(3,3,3-trifluoropropyl)-4b,5,6,7,8,8a(R)-9,10-octahydrophenanthrene-2-carboxylic acid (II) with 3-aminomethyl-2-methylpyridine (III) in the presence of carbonyldiimidazole. Thus, II (preparation given) and carbonyldiimidazole were refluxed 2 h in THF; III in THF was added followed by stirring for 3 h at room temperature to give 69% I.

L6 ANSWER 34 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2002:330263 CAPLUS

DN 136:340495

TI Preparation of octahydrophenanthrenyl carbamates as glucocorticoid receptor modulators

IN Liu, Kevin Kun-Chin; Morgan, Bradley Paul; Robinson, Ralph Pelton, Jr.

PA Pfizer Products Inc., USA

SO Eur. Pat. Appl., 42 pp.

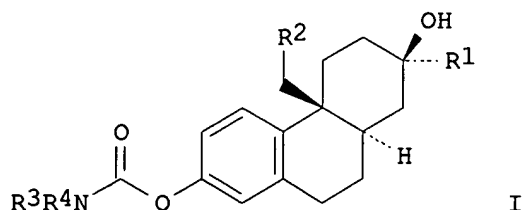
CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1201649	A1	20020502	EP 2001-309064	20011025
	EP 1201649	B1	20060531		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2002193911	A2	20020710	JP 2001-328050	20011025
	CA 2360308	AA	20020428	CA 2001-2360308	20011026
	CA 2360308	C	20060207		
	US 2002107235	A1	20020808	US 2001-6215	20011026
	BR 2001004831	A	20020820	BR 2001-4831	20011026
PRAI	US 2000-243993P	P	20001028		
OS	MARPAT 136:340495				
GI					



AB Title compds. [I; R1 = (trifluoromethyl)alkyl, CF<sub>3</sub>, C.tplbond.CMe, C.tplbond.CCl, C.tplbond.CCF<sub>3</sub>, CH<sub>2</sub>OA; A = (trifluoromethyl)alkyl; R2 = alkyl, alkenyl, (substituted) Ph; R3 = H, alkyl, haloalkyl, alkenyl, alkynyl, haloalkynyl; R4 = H, alkylamino, alkylhet; R3R4N = het; het = (substituted) 5-7 membered (unsatd.) heterocyclic ring containing 1-3 of N, O, S; and including any bicyclic group in which any of the above heterocyclic rings is fused to a benzene ring or another heterocyclic ring; and optionally substituted with 1-4 R7; R7 = (substituted) alkyl; with provisos], were prepared for treatment of obesity, diabetes, depression, anxiety, neurodegeneration, and inflammatory disease (no data). A solution of 2,7-phenanthrenediol, 1,2,3,4,4a,9,10,10a-octahydro-4a-(phenylmethyl)-2-ethyl-[2R-(2 $\alpha$ ,4 $\alpha$ ,10 $\alpha$ )] (preparation given), COCl<sub>2</sub>, and Et<sub>3</sub>N in THF was stirred at room temperature for 3 h; 1-(2-aminoethyl)pyrrolidine was added followed by stirring overnight to give 41% carbamic acid, [2-(1-pyrrolidinyl)ethyl]-, (4bS,7R,8aR)-7-ethyl-4b,5,6,7,8,8a,9,10-octahydro-7-hydroxy-4b-(phenylmethyl)-2-phenanthrenyl ester.

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 35 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2002:86132 CAPLUS

DN 136:332658

TI Scandium ion-promoted photoinduced electron transfer oxidation of fullerenes by p-benzoquinones

AU Fukuzumi, Shunichi; Mori, Hisahiro; Imahori, Hiroshi; Suenobu, Tomoyoshi; Araki, Yasuyuki; Ito, Osamu; Kadish, Karl M.

CS Department of Material and Life Science, Graduate School of Engineering, Osaka University, CREST, Japan Science and Technology Corporation (JST), Suita, 565-0871, Japan

SO Proceedings - Electrochemical Society (2001), 2001-11(Fullerenes--Volume 11: Fullerenes for the New Millennium), 27-40

CODEN: PESODO; ISSN: 0161-6374

PB Electrochemical Society

DT Journal

LA English

AB In the presence of scandium triflate, an efficient photoinduced electron transfer from the triplet excited state of C<sub>60</sub> to p-chloranil occurs to produce C<sub>60</sub> radical cation which has a diagnostic NIR (near IR) absorption band at 980 nm. The observed second-order rate constant of electron transfer (ket) increases linearly with increasing scandium ion concentration In contrast

to the case of p-chloranil, the ket value for electron transfer from 3C<sub>60</sub>\* to p-benzoquinone exhibits first-order dependence on [Sc<sup>3+</sup>] at low concns., changing to second-order dependence at high concns. Such a mixture of first-order and second-order dependence on [Sc<sup>3+</sup>] is also observed for a Sc<sup>3+</sup>-promoted electron transfer from CoTPP (TPP<sup>2-</sup> = tetraphenylporphyrin dianion) to p-benzoquinone. This is ascribed to formation of 1:1 and 1:2

complexes between semiquinone radical anion and  $\text{Sc}^{3+}$  at low and high concns. of  $\text{Sc}^{3+}$ , resp., which results in acceleration of the rate of electron transfer. The  $\text{Sc}^{3+}$ -promoted electron transfer rate consts. have been determined for photoinduced electron transfer from the triplet excited states of C60 derivs. as well as higher fullerenes and the values are compared with the ionization potentials of these fullerene derivs.

RE.CNT 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 36 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2001:848926 CAPLUS  
DN 136:119162  
TI Preparation and characterization of a new solvent-free polymer electrolyte based on spiroketal structure  
AU Tsutsumi, Hiromori; Shirotani, Rumiko; Onimura, Kenjiro; Oishi, Tsutomu  
CS Department of Applied Chemistry and Chemical Engineering, Faculty of Engineering, Yamaguchi University, Yamaguchi, 755-8611, Japan  
SO Electrochemical and Solid-State Letters (2001), 4(12), A195-A196  
CODEN: ESLEF6; ISSN: 1099-0062  
PB Electrochemical Society  
DT Journal  
LA English  
AB Solvent-free solid polymer electrolytes based on spiropolymers were prepared and their properties were confirmed by conductance, differential scanning calorimetry, and X-ray diffraction measurements. The spiropolymer was synthesized from the bicyclic diketone and pentaerythritol. The spiro-polyketal (SP) dissolves lithium perchlorate and the conductivity of the  $(\text{SP})_1.5(\text{LiClO}_4)_1$  complex is  $4.24 + 10^{-5} \text{ S cm}^{-1}$  at  $30^\circ$  and  $3.83 + 10^{-4} \text{ S cm}^{-1}$  at  $60^\circ$ .

RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 37 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2001:847183 CAPLUS  
DN 136:142421  
TI Scandium Ion-Promoted Photoinduced Electron-Transfer Oxidation of Fullerenes and Derivatives by p-Chloranil and p-Benzoquinone  
AU Fukuzumi, Shunichi; Mori, Hisahiro; Imahori, Hiroshi; Suenobu, Tomoyoshi; Araki, Yasuyuki; Ito, Osamu; Kadish, Karl M.  
CS Department of Material and Life Science Graduate School of Engineering, Osaka University CREST, Japan Science and Technology Corporation (JST), Suita, Osaka, 565-0871, Japan  
SO Journal of the American Chemical Society (2001), 123(50), 12458-12465  
CODEN: JACSAT; ISSN: 0002-7863  
PB American Chemical Society  
DT Journal  
LA English  
AB In the presence of scandium triflate, an efficient photoinduced electron transfer from the triplet excited state of C60 to p-chloranil occurs to produce C60 radical cation which has a diagnostic NIR (near-IR) absorption band at 980 nm, whereas no photoinduced electron transfer occurs from the triplet excited state of C60 ( $3\text{C}60^*$ ) to p-chloranil in the absence of scandium ion in benzonitrile. The electron-transfer rate obeys pseudo-first-order kinetics and the pseudo-first-order rate constant increases linearly with increasing p-chloranil concentration. The observed second-order rate constant of electron transfer (ket) increases linearly with increasing scandium ion concentration. In contrast to the case of the C60/p-chloranil/ $\text{Sc}^{3+}$  system, the ket value for electron transfer from



3C60\* to p-benzoquinone increases with an increase in Sc3+ concentration ([Sc3+])

to exhibit a first-order dependence on [Sc3+], changing to a second-order dependence at the high concns. Such a mixture of first-order and second-order dependence on [Sc3+] is also observed for a Sc3+-promoted electron transfer from CoTPP (TPP2- = tetraphenylporphyrin dianion) to p-benzoquinone. This is ascribed to formation of 1:1 and 1:2 complexes between the generated semiquinone radical anion and Sc3+ at the low and high concns. of Sc3+, resp. The transient absorption spectra of the radical cations of various fullerene derivs. were detected by laser flash photolysis of the fullerene/p-chloranil/Sc3+ systems. The ESR spectra of the fullerene radical cations were also detected in frozen PhCN at 193 K under photoirradn. of the fullerene/p-chloranil/Sc3+ systems. The Sc3+-promoted electron-transfer rate consts. were determined for photoinduced electron transfer from the triplet excited states of C60, C70, and their derivs. to p-chloranil and the values are compared with the HOMO (HOMO) levels of the fullerenes and their derivs.

RE.CNT 68 THERE ARE 68 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 38 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2001:338070 CAPLUS

DN 134:336224

TI Use of corticotropin releasing factor (CRF) antagonists for treating syndrome X

IN Chen, Yuhpyng Liang; Hamanaka, Ernest Seiichi

PA Pfizer Products Inc., USA

SO Eur. Pat. Appl., 55 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1097709	A2	20010509	EP 2000-309441	20001026
	EP 1097709	A3	20051221		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
	AU 776724	B2	20040916	AU 2000-66695	20001024
	ZA 2000006008	A	20020426	ZA 2000-6008	20001026
	US 6589947	B1	20030708	US 2000-696822	20001026
	CA 2325069	AA	20010429	CA 2000-2325069	20001027
	NZ 507825	A	20041126	NZ 2000-507825	20001027
PRAI	US 1999-162340P	P	19991029		

OS MARPAT 134:336224

AB Compns. and methods are provided for achieving a therapeutic effect, including the treatment or prevention of syndrome X in an animal, preferably a mammal including a human subject or a companion animal, using a CRF antagonist alone or together with a glucocorticoid receptor antagonist.

L6 ANSWER 39 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2001:136227 CAPLUS

DN 134:340801

TI Photochemical Generation of Polymeric Alkyl-C60 Radicals: ESR Detection and Identification

AU Qu, Baojun; Hawthorn, Geoff; Mau, Albert W. H.; Dai, Liming

CS State Key Laboratory of Fire Science and Department of Polymer Science and

Engineering, University of Science and Technology of China, Hefei Anhui, 230026, Peop. Rep. China

SO Journal of Physical Chemistry B (2001), 105(11), 2129-2134  
CODEN: JPCBFK; ISSN: 1089-5647

PB American Chemical Society

DT Journal

LA English

AB ESR spectroscopy has been used to study various alkylfullerene radical adducts generated by UV-photoinitiated reactions between low-d. polyethylene (LDPE) and C60 in the presence or absence of benzophenone (BP) as a photoinitiator under different conditions. Photolysis of LDPE/BP/C60 mixture in toluene at 323 K produced benzylfullerene (RC60) radical adducts, showing a strong ESR signal of  $g = 2.00270$  with several well-resolved pairs of  $^{13}\text{C}$  satellites. On the other hand, a well-resolved ESR spectrum characteristic of polymeric alkylfullerene (PC60) radical adducts was observed during UV irradiation of the LDPE/BP/C60 in benzene or in the molten state (413 K). Detailed analyses of hyperfine structures (hfs) revealed that the ESR spectrum for PC60 radical adducts consisted of three components: (1) a broad singlet at  $g = 2.00250$  arising from C60 radical anions; (2) an innermost pair of  $^{13}\text{C}$  satellites; and (3) a 12-line spectrum superimposed on the broad singlet. Spectroscopic simulation allowed the 12-line spectrum to be attributed to the coexistence of two polymeric radical adducts of C60 (i.e., the tertiary carbon radical adduct,  $-(\text{CH}_2)_3\text{C}-\text{C}_{60}^\bullet$ , designated as PAC60 $^\bullet$ , and the secondary carbon radical adduct,  $-(\text{CH}_2)_2\text{CH}-\text{C}_{60}^\bullet$ , designated as PBC60 $^\bullet$ ), which have slightly different  $g$  values ( $g_A = 2.00248$  and  $g_B = 2.00244$ ) and integral intensities IA/IB (48.4/51.6). These results clearly indicated the generation of C60-bonded LDPE materials simply by photoirradn. of LDPE/C60 with BP as a photoinitiator.

RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 40 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2001:88082 CAPLUS

DN 134:246396

TI Effects of lowering symmetry on the ESR spectra of radical anions of fullerene derivatives

AU Fukuzumi, Shunichi; Mori, Hisahiro; Suenobu, Tomoyoshi; Imahori, Hiroshi; Gao, Xiang; Kadish, Karl M.

CS Department of Material and Life Science, Graduate School of Engineering, Osaka University, CREST, JAPAN Science and Technology Corporation, Suita, 565-0871, Japan

SO Proceedings - Electrochemical Society (2000), 2000-10(Fullerenes 2000--Volume 8: Electrochemistry and Photochemistry), 18-30  
CODEN: PESODO; ISSN: 0161-6374

PB Electrochemical Society

DT Journal

LA English

AB Radical anions of dibenzyl adducts of C60, 1,4-(C6H5CH2)2C60 $^{\bullet-}$  and 1,2-(C6H5CH2)2C60 $^{\bullet-}$ , give ESR spectra which have larger  $g$  values (2.0004 and 2.0001, resp.) and much smaller linewidths ( $\Delta H_{\text{msl}} = 2.5$  and 3.9 G, resp. at 213 K) than the  $g$  value (1.9984) and the  $\Delta H_{\text{msl}}$  value (30.9 G at 213 K) of C60 $^{\bullet-}$ . An even smaller  $\Delta H_{\text{msl}}$  value (0.17 G) and a larger  $g$  value (2.0011) are observed in the tetrabenzyl C60 adduct radical anion, 1,4,10,24-(C6H5CH2)4C60 $^{\bullet-}$ . This is ascribed to a large splitting of the degenerate tlu orbitals caused by introduction of four benzyl groups to C60. In this case, a hyperfine structure, due to two nonequivalent protons of only one benzyl group ( $a_{\text{H1}}$

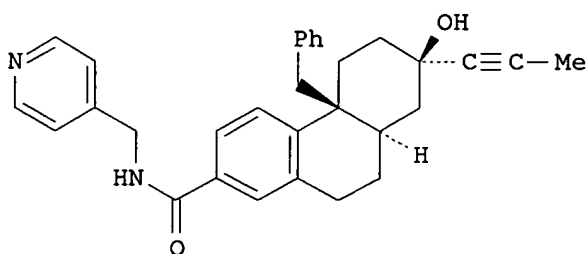
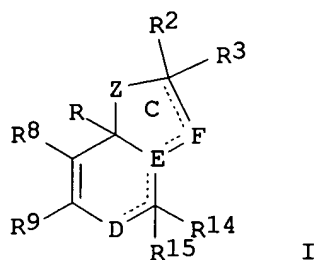
= 0.31 G,  $a_{H2} = 0.11$  G), is observed and this is consistent with the predicted localized spin d. at the C2 position next to the C1 carbon to which a benzyl group is attached. The radical anions of the mono- and bisadducts formed in the Diels-Alder cycloaddn. reaction of C60 with 9,10-dimethylantracene show ESR signals at different g values (2.0003 for the monoadduct and 2.0009 for the bisadduct). The relation between lower symmetry and the ESR spectra of radical anions of various C60 derivs. is discussed based on the change in the g values and the linewidths. The energy gap ( $\delta$ ) between the singly occupied orbital and the two other orbitals which had the tlu symmetry prior to introduction of addends to C60 is derived from the difference in the g values of various C60-derivs. from the free spin value (2.0023). There is a linear correlation between  $\log \Delta H_{msl}$  and  $-\delta$ .

RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 41 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2000:790448 CAPLUS  
DN 133:350060  
TI Preparation of nonracemic octahydrophenanthrene and other tricyclic  
derivs. as selective modulators of glucocorticoid receptors  
IN Dow, Robert Lee; Liu, Kevin Kun-Chin; Morgan, Bradley Paul; Swick, Andrew  
Gordon  
PA Pfizer Products Inc., USA  
SO PCT Int. Appl., 279 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000066522	A1	20001109	WO 2000-IB366	20000327
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	CA 2372173	AA	20001109	CA 2000-2372173	20000327
	BR 2000010138	A	20020122	BR 2000-10138	20000327
	EP 1175383	A1	20020130	EP 2000-911172	20000327
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	TR 200103104	T2	20020521	TR 2001-3104	20000327
	JP 2002543169	T2	20021217	JP 2000-615356	20000327
	EE 200100567	A	20030217	EE 2001-567	20000327
	NZ 514465	A	20031128	NZ 2000-514465	20000327
	AU 776608	B2	20040916	AU 2000-33165	20000327
	CN 1781890	A	20060607	CN 2005-10128846	20000327
	US 6380223	B1	20020430	US 2000-559384	20000427
	ZA 2001008846	A	20021028	ZA 2001-8846	20011026
	NO 2001005272	A	20011228	NO 2001-5272	20011029
	HR 2001000804	A1	20021231	HR 2001-804	20011030
	BG 106142	A	20020531	BG 2001-106142	20011123
	US 2002147336	A1	20021010	US 2002-80174	20020219
	US 6699893	B2	20040302		

	US 2003199527	A1	20031023	US 2003-413879	20030415
	US 6777404	B2	20040817		
	US 2004176595	A1	20040909	US 2003-721318	20031125
PRAI	US 1999-132130P	P	19990430		
	US 1999-162340P	P	19991029		
	CN 2000-806949	A3	20000327		
	WO 2000-IB366	W	20000327		
	US 2000-559384	A3	20000427		
	US 2000-696822	A3	20001026		
	US 2002-80174	A1	20020219		
OS	MARPAT 133:350060				
GI					



AB Title compds. [e.g., I; D = CR7, CR7R16, N, NR7, O' E = C, CR6, N; F = CR4, CR4R5, O; R = XR1; R1 = H, alkyl, acylalkyl, arylalkyl, etc.; R2 = H, halo, alkyl, alkoxy, etc.; R3 = H, alkyl, arylalkyl, etc.; 1 of R2,R3 = null when adjacent dashed line = bond; R4,R5 = H, cyano, alkyl, alkoxy, etc.; R4R5 = O; R6 = H, cyano, alkyl, alkoxy, OH, etc.; R7,R16 = H, halo, cyano, alkyl, etc.; R7R16 = O; R8R9 = atoms to complete a substituted heteroarom. ring; R14,R15 = H, halo, alkyl, alkoxy, etc.; R14R15 = O when adjacent dashed lines = null; X = bond, CH2, CH(OH), CO; Z = (un)substituted CH2, -CH2CH2, -CH2CO, CO, etc.; dashed lines = optional bonds] were prepared as glucocorticoid receptor modulators (no data). E.g., 6-methoxy-2-tetralone was alkylated by formation of the pyrrolidine enamine and alkylation with benzyl bromide; the benzylated ketone then undergoes asym. Michael addition with Me vinyl ketone in the presence of (S)-(-)- $\alpha$ -methylbenzylamine followed by cyclocondensation with sodium methoxide to give a nonracemic methoxytetrahydrophenanthrenone derivative. E.g., demethylation of the methoxytetrahydrophenanthrenone with boron trichloride, reduction of the enone with lithium and ammonia, addition of 1-lithiopropyne to the ketone, formation of the aryl triflate with triflic anhydride and carbonylation with carbon monoxide in the presence in the presence of palladium acetate and bis(diphenylphosphino)propanol gives an

hydroxyoctahydrophenanthrenecarboxylic acid derivative which is coupled with 4-(aminomethyl)pyridine in the presence of trimethylaluminum to give the octahydrophenanthrenecarboxamide II as one of the title compds.

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 42 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2000:745440 CAPLUS  
DN 134:29098  
TI Effects of Lowering Symmetry on the ESR Spectra of Radical Anions of Fullerene Derivatives and the Reduction Potentials  
AU Fukuzumi, Shunichi; Mori, Hisahiro; Suenobu, Tomoyoshi; Imahori, Hiroshi; Gao, Xiang; Kadish, Karl M.  
CS Department of Material and Life Science Graduate School of Engineering, Osaka University CREST Japan Science and Technology Corporation, Suita Osaka, 565-0871, Japan  
SO Journal of Physical Chemistry A (2000), 104(46), 10688-10694  
CODEN: JPCAFH; ISSN: 1089-5639  
PB American Chemical Society  
DT Journal  
LA English  
AB Radical anions of dibenzyl adducts of C<sub>60</sub>, 1,4-(C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>2</sub>C<sub>60</sub>•- and 1,2-(C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>2</sub>C<sub>60</sub>•-, give ESR spectra which have larger g values (2.0004 and 2.0001, resp.) and much smaller line widths ( $\Delta H_{msl}$  = 2.5 and 3.3 G, resp., at 213 K) than the g value (1.9984) and the  $\Delta H_{msl}$  value (30.9 G at 213 K) of C<sub>60</sub>•-. An even smaller  $\Delta H_{msl}$  value (0.17 G) and a larger g value (2.0011) are observed for the tetrabenzyl C<sub>60</sub> adduct radical anion, 1,4,10,24-(C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>4</sub>C<sub>60</sub>•- and this is ascribed to a large splitting of the degenerate t<sub>1u</sub> orbitals caused by introduction of four benzyl groups to C<sub>60</sub>. In this case, a hyperfine structure, due to two nonequivalent protons of only one benzyl group (aH<sub>1</sub> = 0.31 G, aH<sub>2</sub> = 0.11 G), is observed and this is consistent with the predicted localized spin d. at the C<sub>2</sub> position next to the C<sub>1</sub> carbon to which a benzyl group is attached. The radical anions of the mono- and bisadducts formed in the Diels-Alder cycloaddn. reaction of C<sub>60</sub> with 9,10-dimethylantracene show ESR signals at different g values (2.0003 for the monoadduct and 2.0009 for the bisadduct). The relationship between lower symmetry and the ESR spectra of radical anions of various C<sub>60</sub> derivs. is discussed in terms of the g values and the line widths. The energy gap ( $\delta$ ) between the singly occupied orbital and the two other orbitals which had a t<sub>1u</sub> symmetry prior to introduction of addends to C<sub>60</sub> is derived from differences in the g values of various C<sub>60</sub>•- derivs. from the free spin value (2.0023). A linear correlation is shown to exist between log  $\Delta H_{msl}$  and - $\delta$ . The  $\delta$  values are also obtained from Arrhenius plots of ln  $\Delta H_{msl}$  vs T<sup>-1</sup> and they agree well with the values derived from the g values and the reduction potentials.

RE.CNT 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 43 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2000:601308 CAPLUS  
DN 133:266381  
TI Photoalkylation of C<sub>60</sub> by alkylcobalt(III) complexes  
AU Ohkubo, Kei; Fukuzumi, Shunichi  
CS Department of Material and Life Science, Graduate School of Engineering, Osaka University, CREST, JAPAN Science and Technology Corporation, Suita, 565-0871, Japan  
SO Inorganic Reaction Mechanisms (Amsterdam) (2000), 2(1-2), 147-153

CODEN: IRMEFE; ISSN: 1028-6624

PB Gordon &amp; Breach Science Publishers

DT Journal

LA English

AB Photolysis of a benzonitrile solution of alkylcobalt(III) complexes, [RCo(DH)2py] (R = Me and PhCH<sub>2</sub>, (DH)<sub>2</sub> = bis(dimethylglyoximate), py = pyridine) in the presence of C<sub>60</sub> by using visible light results in alkylation of C<sub>60</sub> to yield R<sub>2</sub>C<sub>60</sub>. The excited state of [RCo(DH)2py] rather than C<sub>60</sub> is responsible for the photoalkylation of C<sub>60</sub>, since the action spectrum for formation of R<sub>2</sub>C<sub>60</sub> agrees with the absorption spectrum of [RCo(DH)2py] which is quite different from that of C<sub>60</sub>. The photoalkylation of C<sub>60</sub> is retarded by a radical trapping reagent such as 2,2,6,6-tetramethyl-1-piperidinyloxy radical (TEMPO). This indicates that photoalkylation of C<sub>60</sub> proceeds via photocleavage of the cobalt-carbon bond of [RCo(DH)2py]. The intermediate benzyl radical produced by the photocleavage reaction of [PhCH<sub>2</sub>Co(DH)2py] is detected by ESR.

RE.CNT 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 44 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2000:359956 CAPLUS

DN 133:135092

TI Stepwise Synthesis of Fullerene Cyclopentadienide R<sub>5</sub>C<sub>60</sub>- and Indenide R<sub>3</sub>C<sub>60</sub>-. An Approach to Fully Unsymmetrically Substituted Derivatives

AU Sawamura, Masaya; Toganoh, Motoki; Suzuki, Kazuhiro; Hirai, Atsushi; Iikura, Hitoshi; Nakamura, Eiichi

CS Department of Chemistry, The University of Tokyo, Tokyo, 113-0033, Japan

SO Organic Letters (2000), 2(13), 1919-1921

CODEN: ORLEF7; ISSN: 1523-7060

PB American Chemical Society

DT Journal

LA English

OS CASREACT 133:135092

AB Fullerene cyclopentadienide (PhCH<sub>2</sub>)<sub>2</sub>Ph<sub>3</sub>C<sub>60</sub>- and indenide (PhCH<sub>2</sub>)<sub>2</sub>PhC<sub>60</sub>-, each bearing two different organic groups, were efficiently synthesized through regioselective reactions of 1,4-(PhCH<sub>2</sub>)<sub>2</sub>C<sub>60</sub> with an organocopper reagent (PhMgBr/CuBr.SMe<sub>2</sub>) or a Grignard reagent (PhMgBr) followed by deprotonation with KOCMe<sub>3</sub>.

RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 45 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2000:355978 CAPLUS

DN 133:58486

TI CIDEP Studies of Fullerene-Derived Radical Adducts

AU Koptug, Igor V.; Goloshevsky, Artem G.; Zavarine, Igor S.; Turro, Nicholas J.; Krusic, Paul J.

CS International Tomography Center, Novosibirsk, Russia

SO Journal of Physical Chemistry A (2000), 104(24), 5726-5731

CODEN: JPCAFH; ISSN: 1089-5639

PB American Chemical Society

DT Journal

LA English

AB Photolyses of solns. containing organomercury compds. (HgR<sub>2</sub>) in the presence of C<sub>60</sub> fullerene have been investigated by Fourier transform time-resolved EPR (FT TR EPR) and continuous-wave EPR (CW EPR) techniques. By FT TR EPR, both electron-spin-polarized 3C<sub>60</sub> (A polarization) and

electron-spin-polarized adducts •C60R (E/A + E polarization) are observed. The CW EPR spectra of the •C60R radicals under steady-state irradiation also exhibit some electron-spin polarization. The chemical induced dynamic electron polarization (CIDEP) in the FT TR EPR expts. is explained by the following series of steps. Photolysis initially causes cleavage of the organomercury compds. into radicals that add to C60 to form •C60R. The latter combine to form the dimers, [C60R]2, which are thermally stable and accumulate in the samples. In all of the reported expts., a certain quantity of dimers is produced by photolysis before the EPR spectra are acquired. In the FT TR EPR expts., laser excitation produces 3C60 by excitation of C60 and •C60R by photocleavage of the dimers. The observed E/A CIDEP patterns at short (<1 μs) delays after the laser flash are proposed to be a result of the creation of polarization through the radical-pair mechanism (RPM) resulting from the interactions of two •C60R radicals (geminate or free) formed from the photocleavage of [C60R]2 dimers. The addnl. E polarization observed at later times (>1 μs) is proposed to result from the interaction of 3C60 with •C60R radicals, creating E polarization through the radical-pair-triplet mechanism (RPTM). The polarization observed in the CW EPR expts. is attributed to the maintenance of polarization through the radical lifetime because of the extremely long spin-lattice relaxation of the •C60R radicals. The latter conclusion is consistent with the very small (50 mG) line widths of the adduct radicals. An upper limit for the bond energy of the [C60R]2 dimers of 226 kJ/mol is established by the observation of the CIDEP of •C60R radicals when 532-nm excitation is employed. The role of multiple adducts in the observed FT TR EPR spectra is discussed.

RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 46 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2000:205506 CAPLUS

DN 132:334150

TI Effect of Addition Pattern on the Electrochemical and Spectroscopic Properties of Neutral and Reduced 1,2- and 1,4-(C6H5CH2)2C60 Isomers

AU Kadish, Karl M.; Gao, Xiang; Van Caemelbecke, Eric; Suenobu, Tomoyoshi; Fukuzumi, Shunichi

CS Department of Chemistry, University of Houston, Houston, TX, 77204-5641, USA

SO Journal of Physical Chemistry A (2000), 104(17), 3878-3883

CODEN: JPCAFH; ISSN: 1089-5639

PB American Chemical Society

DT Journal

LA English

AB The spectral and electrochem. properties of isomeric 1,2- and 1,4-adducts of fullerenes R2C60 were examined in their neutral, singly and/or doubly reduced forms. The 1st reduction potentials of 1,2- and 1,4-(C6H5CH2)2C60 in PhCN containing 0.1M TBAP are the same within exptl. error but the 2nd and 3rd redns. of the 2 isomers differ by 50 mV, with the 1,2-isomer being easier to reduce. Much larger differences, however, are seen in the near-IR spectra of the singly and doubly reduced organofullerene isomers. The monoanion of 1,2-R2C60 possesses an absorption band at .apprx.1000 nm, while the dianion has a band at .apprx.900 nm. The 1,4-R2C60 derivs. also show bands at similar wavelengths in their monoanionic and dianionic forms, but there is a 2nd near-IR band at 1500 (monoanion) or 1300 nm (dianion).

RE.CNT 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 47 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2000:150054 CAPLUS

DN 132:278876

TI Splitting of Degenerate Orbitals of Dibenzyl and Tetrabenzyl Adducts of C60: ESR of the Radical Anions and the Rotation Barriers of Benzyl Groups

AU Fukuzumi, Shunichi; Suenobu, Tomoyoshi; Gao, Xiang; Kadish, Karl M.

CS Department of Material and Life Science Graduate School of Engineering, CREST, Japan Sci. Technol. Corp., Osaka University, Suita, Osaka, 565-0871, Japan

SO Journal of Physical Chemistry A (2000), 104(13), 2908-2913

CODEN: JPCAFH; ISSN: 1089-5639

PB American Chemical Society

DT Journal

LA English

AB The degenerate 2E<sub>1u</sub> ground state and the thermally accessible low-lying 2A<sub>2u</sub> excited state of C60<sup>•-</sup> give a broad ESR signal ( $\Delta H_{msl}$  = 30.9 G at 213 K) which has a smaller g value (1.9984) as compared to the free spin value (2.0023) and linewidth which decreases with decreasing temperature ( $\Delta H_{msl}$  = 6.5 G at 133 K). The 1h symmetry of the parent C60 is lowered by the introduction of two benzyl groups to C60 to give 1,4-(C6H5CH2)2C60, which leads to the larger g value (2.0004) of 1,4-(C6H5CH2)2C60<sup>•-</sup> than that of C60<sup>•-</sup> (g = 1.9984) and a much smaller linewidth ( $\Delta H_{msl}$  = 2.5 G at 213 K) which is independent of temperature. An even smaller  $\Delta H_{msl}$  value (0.17 G) and a larger g value (2.0011) are observed in the tetrabenzyl C60 adduct radical anion, 1,4,10,24-(C6H5CH2)4C60<sup>•-</sup>. This is ascribed to a large splitting of the degenerate t<sub>1u</sub> orbitals caused by introduction of four benzyl groups to C60. In this case, a hyperfine structure due to two nonequivalent protons of only one benzyl group (aH1 = 0.31 G, aH2 = 0.11 G) is observed and this is consistent with the predicted localized spin d. at the C2 position next to the C1 carbon to which a benzyl group is attached. The observation of two nonequivalent hyperfine coupling consts. due to the benzyl methylene protons indicates that rotation of the benzyl group at the C1 position is slow on the ESR time scale. The slow rotation rates of the benzyl groups in 1,4-dibenzyl adducts of C60 and the activation parameters were determined from a line broadening of the methylene protons in the 1H NMR spectra with increasing temperature

RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 48 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2000:150053 CAPLUS

DN 132:264799

TI Electrogeneration and Characterization of (C6H5CH2)2C70

AU Kadish, Karl M.; Gao, Xiang; Gorelik, Olga; Van Caemelbecke, Eric; Suenobu, Tomoyoshi; Fukuzumi, Shunichi

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SO Journal of Physical Chemistry A (2000), 104(13), 2902-2907

CODEN: JPCAFH; ISSN: 1089-5639

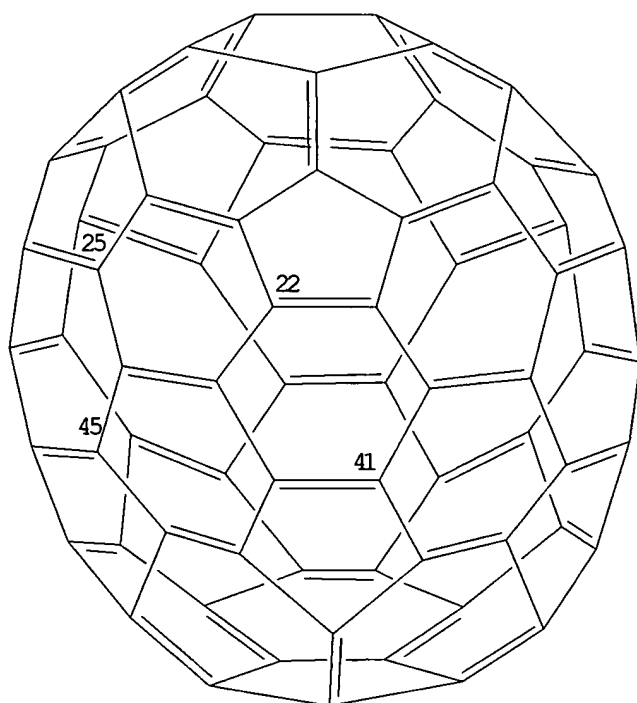
PB American Chemical Society

DT Journal

LA English

GI





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AB (C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>2</sub>C<sub>70</sub> was electrosynthesized from C<sub>70</sub><sup>2-</sup> and C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>Br and purified by HPLC. Mass spectral results for the largest HPLC fraction confirm formation of the compound, while <sup>1</sup>H NMR spectroscopy suggests that three isomers are present in this fraction, all of which are 1,4-addition products. The isomers are proposed to be the 22,25-, 22,41-, and 22,45-isomers (see locant labels on I) on the basis of <sup>1</sup>H NMR data and the fact that bulky benzyl groups on C<sub>60</sub> form preferentially 1,4- rather than 1,2-addition products. (C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>2</sub>C<sub>70</sub> was examined as to its electrochem. properties, and two sets of reduction processes were observed, one of which is assigned to the 22,25- and 22,41-isomers that exhibit identical electrochem. properties and the other to the 22,45-isomer of (C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>2</sub>C<sub>70</sub>. The vis-near-IR spectrum of (C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>2</sub>C<sub>70</sub><sup>•-</sup> in benzonitrile shows a strong band at 776 nm which is not seen for C<sub>70</sub><sup>•-</sup> as well as two more bands in the near-IR region (1062 and 1250 nm) which are blue-shifted with respect to the near-IR absorption band of C<sub>70</sub><sup>•-</sup> that appears at 1368 nm.

RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD  
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L6 ANSWER 49 OF 49 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2000:22117 CAPLUS  
DN 132:222329  
TI Electrosynthesis and Structural Characterization of Two (C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>4</sub>C<sub>60</sub> Isomers  
AU Kadish, Karl M.; Gao, Xiang; Van Caemelbecke, Eric; Suenobu, Tomoyoshi; Fukuzumi, Shunichi  
CS Department of Chemistry, University of Houston, Houston, TX, 77204-5641, USA  
SO Journal of the American Chemical Society (2000), 122(4), 563-570  
CODEN: JACSAT; ISSN: 0002-7863  
PB American Chemical Society  
DT Journal

LA English

AB The structural, spectral, and electrochem. properties of two (C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>4</sub>C<sub>60</sub> isomers are reported. One is designated as the 1,4;1,4-(C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>4</sub>C<sub>60</sub> isomer and the other as the 1,4;1,2-isomer of (C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>4</sub>C<sub>60</sub>. The two isomers were isolated by HPLC from the products obtained by a reaction between [(C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>2</sub>C<sub>60</sub>]<sup>2-</sup> and C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>Br. X-ray data show that the two (C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>4</sub>C<sub>60</sub> isomers differ from one another by the position of only one benzyl group and that, in each compound, the four benzyl addends are in close proximity. Both (C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>4</sub>C<sub>60</sub> isomers undergo three one-electron redns. in PhCN containing 0.1 M tetrabutylammonium perchlorate (TBAP) and have E<sub>1/2</sub> values which are more neg. than values for either C<sub>60</sub> or 1,4-(C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>2</sub>C<sub>60</sub>. The mono-anions of 1,4;1,4- and 1,4;1,2-(C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>)<sub>4</sub>C<sub>60</sub> were electrogenerated by bulk controlled-potential electrolysis in PhCN containing 0.2 M TBAP and characterized as to their spectral properties in both the visible and near-IR regions.

RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD  
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SINCE FILE	TOTAL
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